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MEMORANDUM REPORT ARBRL-MR-03362

A MEFF USER'S GUIDE

George E. Keller

July 1984

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US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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The Yousefian flash prediction model, which includes the Muzzle Exhaust Flow Field (MEFF) program, is the only operational flash prediction model for guns that takes detailed chemistry into account. This report provides a well-described path for intelligent application of the Yousefian flash prediction model. A sample calculation is followed from beginning to end, and all input and output are discussed thoroughly.

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TABLE OF CONTENTS

I. INTRODUCTION

Secondary muzzle flash results from the reignition of hot, fuel-rich gun muzzle exhaust gases when they mix with air after the gun projectile is launched. Secondary muzzle flash has several deleterious effects, so that there have been continuing efforts to learn to model, predict, and suppress it. The Yousefian flash prediction model, which includes the Muzzle Exhaust Flow Field (MEFF) program[1], is the only operational flash prediction model that takes detailed chemistry into account. If one wants to predict the effect of a new suppressant combination or of a new propellant composition, the Yousefian model is the only game in town.

The name MEFF is used by its author to describe both the front-end program which models the gun muzzle exhaust flow field and the overall modeling procedure, which includes the Low-Altitude Plume Prediction (LAPP) model.[2] LAPP contains the detailed chemical modeling; and MEFF was written to produce rational input parameters for LAPP in a fashion that changes appropriately with changes in gun parameters. MEFF is a "gun input" to LAPP, if you would. In this report, I shall attempt to confine my use of the name MEFF to descriptions of the muzzle exhaust flow field program, with the term "Yousefian model" used to describe MEFF, LAPP, and their associated programs.

The physics described by MEFF is well documented, and the reader is referred to Reference 1 for questions concerning the reasons MEFF is written the way it is. MEFF starts with the equations derived by Corner;[3] one resulting limitation of the code is that it is limited to cases for which the charge weight is significantly less than the projectile weight. Thus, MEFF cannot be used to model most high-velocity guns, such as those on tanks.

There are several discrete steps involved in using the Yousefian model, and not all of them are obvious. This report is intended to provide a well-described path for intelligent MEFF/LAPP utilization; one should be able to get the desired results correctly and quickly by following this guide. As an aid to understanding, a sample calculation is followed from beginning to end, and all the input and output are discussed thoroughly.

Four programs are essential to the Yousefian model. First, one needs a thermodynamics code; BLAKE[4] is used throughout this report, but NASA-LEWIS

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1. V. Yousefian, "Muzzle Flash Onset," ARI-RR-236, Aerodyne Research, Inc., Billerica, MA, November 198Ø. Also available as ARBRL-CR-ØØ477, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, February 1982 (AD BØ63 573L).

2. R. R. Mikatarian, C. J. Kau, and H. S. Pergament, "A Fast Computer Program for Nonequilibrium Rocket Plume Predictions," AFRPL-TR-72-94, Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, CA, August 1972.

3. J. Corner, <u>Theory of Interior Ballistics of Guns</u>, John Wiley & Sons, New York (195Ø).

4. E. Freedman, "BLAKE - A Thermodynamic Code Based on TIGER: User's Guide and Manual," ARBRL-TR-Ø2411, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1982 (AD A121 259).

could have been used. This report contains enough details for an experienced BLAKE user to get the desired results; a novice will probably have to get help using BLAKE. The thermodynamics code is used twice, for two separate functions. Second, an interior ballistics code is used; I have here used IBHVG, a modern version of the Baer-Frankle lumped-parameter model.[5] This report contains enough details for an occasional IBHVG user to get the desired results; a novice will have to get help running IBHVG. MEFF is needed as the third major step, and the information in this report is intended to be sufficient to run MEFF. Finally, LAPP[2] is needed; and again, the information in this report should be all a user needs to use LAPP for this application.

For ease in doing MEFF calculations, I wrote two short linking programs, MTOB and CONCEN. They enabled automation of MEFF calculations to the maximum extent practicable.

II. PRELIMINARY THERMOCHEMICAL CALCULATION

Required Results of the Calculation: First of all, one must input appropriate propellant data into a thermodynamics code. The needed output are the quantities required by the interior ballistic code and by MEFF to follow.

Here, IBHVG will be used for the interior ballistic code, so one needs:

Impetus, Adiabatic Flame Temperature, Gamma, and Covolume

For MEFF, one also needs:

Molecular Weight

An Example of the Calculation: The example that has been chosen for this illustrative calculation is for a 155-mm howitzer; and the propellant is the standard M3ØA1 propellant, which contains 1% (by weight) of K_2SO_4 flash suppressant. A listing of the input job stream and data for this calculation is included as Appendix A.

Note the deliberate suppression of many condensed species, e.g., KCO$, KSO$, K$, etc., for the calculations. Since the suppressant is presumed to operate in the gas phase, solid-phase or liquid-phase final constituents that could conceivably tie up some of the potassium were not permitted to be formed in these calculations.

The line which begins with CM2 is the listing of the propellant constituents and the weight percentage of each in the propellant:

NC126Ø	nitrocellulose, 12.6Ø%	27.9Ø% of the total
NG	nitroglycerin	22.42%
NQ	nitroguanidine	46.84%
EC	ethyl centralite	1.49%
KS	potassium sulfate	1.ØØ%

5. P. G. Baer and J. M. Frankle, "The Simulation of Interior Ballistic Performance of Guns by Digital Computer Program," BRL Report No. 1183, U.S. Army Aberdeen Research and Development Center, Ballistic Research Laboratories, Aberdeen Proving Ground, MD, December 1962 (AD 299 98Ø).

ALC	ethyl alcohol	Ø.25%
C	carbon (graphite)	Ø.Ø1%

In this case, a GUN calculation is desired, with the standard loading density of Ø.2 g/cc.

The results of this calculation are shown in detail in Appendix B. The parameter values which carry over directly to the interior ballistic code are:

Impetus	356461 ft-lb/lb
Flame Temperature	3ØØ3 K
Gamma	1.2412
Covolume	28.81 in^3

The values needed for MEFF are:

Molecular Weight	23.432
Covolume	1.Ø41 cc/g

III. INTERIOR BALLISTIC CALCULATION

Input and Output for the Calculation Next, one must use an interior ballistic code. The input parameters needed are:

Chamber volume, length of travel, propellant mass, projectile mass, and barrel cross section

The output quantities muzzle velocity and mean gas temperature at shot ejection are needed by MEFF, as are several of the gun parameters.

An Example of the Calculation: Appendix C is an IBHVG calculation for the example system. System, projectile, and propellant parameters are nominal values for this system. Note the thermodynamic values introduced from the prior BLAKE calculation.

The results of the interior ballistic calculation needed for MEFF are:

Muzzle velocity	265Ø ft/s
Mean gas temp	186Ø K

IV. MEFF CALCULATION

At last one comes to the actual calculation with MEFF itself. The input needed are illustrated by the data on the bottom of the FLASH job stream included as Appendix D. The MEFF listing itself, as modified slightly for automated running, is included as Appendix E. MEFF requirements are as follows:

Data Card	Requirement	Illustrative value
1	A title card	155-MM HOWITZER WITH M2Ø3 CHARGE
2	Muzzle velocity	789 m/s
2	Chamber volume	.Ø1966 m^3
2	Travel	5.Ø8 m

2	Propellant mass	12.23 kg (total of all)
2	Projectile mass	46.36 kg
2	Bore cross section	.Ø192 m^2
2	Gamma	1.243
2	Molecular Weight	23.43
2	Mean gas temperature at shot ejection	1861 K
2	Covolume	.ØØ1Ø46 m^3/kg
3	No. iterations between stored values	4
3	Step size	.ØØ1
3	Init. condition step away from tau=Ø	.Ø1
4	Maximum distance from muzzle for calculation to proceed	5Ø. (meters. 1Ø meters would be appropriate for a mortar calculation.)
4	Print step	5. (meters)
4	Diffusion step size passed to LAPP	.2
4	LAPP output parameter =1, all output =Ø, centerline temperatures only	1

I have never changed the value of the parameters on the third data card. I added the fourth card so it would be easy to vary the weapon-dependent maximum distance from the muzzle for the calculations, the print step, and the diffusion step size. The fourth parameter on the card makes it easy to reduce the voluminous LAPP output to just centerline temperatures, for trouble-shooting. The diffusion step size can be increased, and the run time will be shorter. When one increases the diffusion step size too far, the program will gracefully halt at the moment of ignition. Too large a diffusion step size will not lead to improper results of these calculations.

The output parameters passed from MEFF for calculations to follow are written to TAPE9 at statement 5Ø11, and they are as follows:

TN, the gas temperature at the normal shock when the velocity of the muzzle gas flow becomes sonic

TMØ, the muzzle gas temperature at the time of shot ejection

TB, the gas temperature at the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

PMØ, the muzzle gas pressure at the time of shot ejection

UB, the gas velocity at the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

ALPHA1, the fraction of gas entering the reflected shock

RB, the radius of the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

XMAX, the maximum distance from the muzzle for the calculations, in meters

PRNT, the print step, in meters

FDL, the diffusion step size, passed through for LAPP

KEY, the LAPP output parameter, passed through for LAPP

V. MTOB CALCULATION

Next one prepares for thermodynamic calculations at several different places in muzzle exit gas flow space. MTOB (Appendix F) was written to do this automatically. It takes the MEFF output, combines it with the details of the propellant contained in BOIL (Appendix G), and produces TAPE8, which is a detailed command stream for BLAKE and data for programs CONCEN and LAPP to follow.

VI. BLAKE CALCULATION

Here one needs two thermodynamic calculations, one to calculate the mole fractions at the normal shock, and one to calculate the mole fractions at the reflected shock. The first of these is simply a "point" calculation at the pressure and temperature of the normal shock. For the second, one recalls[1] that the propellant gas expands isotropically from the muzzle to the reflected shock region, so that the mole fractions are the same as those at the muzzle; one thus does a "point" calculation at the pressure and temperature of the muzzle gas as it emerges from the gun.

VII. CONCEN CALCULATION

The program CONCEN (Appendix H) reads the BLAKE output and automatically calculates the mole fraction for each gaseous species at the initial boundary, as shown in Reference 1.

$x_i = (1-\alpha)\, x_n + \alpha\, x_r$, where

x_i is the mole fraction at the initial boundary,
x_n is the mole fraction at the normal shock,
x_r is the mole fraction at the reflected shock, and
α is the fraction of the flow that enters the reflected shock.

Thus, the output of CONCEN or of a calculation by some other means, is a list of the 13 gaseous species that LAPP will consider, and the mole fraction of each, in the exact order that LAPP expects to find them: H_2O, CO, H_2, N_2, CO_2, H, OH, O, O_2, K, KOH, KO_2, HO_2. These results are passed to LAPP on TAPE2.

VIII. LASTDA, THE LAPP STANDARD DATA SET

The file LASTDA contains the standard LAPP input data, including thermodynamic information on the gaseous species allowed and reaction rate data on the reactions considered. The LAPP report[2] documents the needed LAPP input data in detail; here we concentrate on much-used or often-changed data and on changes from the LAPP report. I have used numbers composed of all 9's to "hold the place" of values which will be replaced in a subsequent read, in order to minimize rewriting LAPP.

LAPP Input Card	Source of input	Via	Input
1	FLASH	TAPE8	Title Card
On card 2, all data entered in I5			
2	LASTDA		Initial number of grid points
2	LASTDA		Number of species (24 max); here 13
2	LASTDA		Viscosity option key; 6=Donaldson/Gray
2	LASTDA		Number of reactions; here 25; LAPP has been modified to handle up through 49
2	LASTDA		Three items specifying output options; all Ø
2	LASTDA		Max computer time; never used; here left at 2ØØ
2	LASTDA		Pressure option; never changed; here Ø
2	LASTDA		Number of thermo entries for each species; here 22 and never changed
3	LASTDA		Signal frequencies; left blank since no attenuation calculations are desired
On card 4, all data entered in E1Ø.3			
4	LASTDA		Initial value of X, the distance from the muzzle, in meters.
4	FLASH	TAPE8	Final value of X in meters.
4	FLASH	TAPE8	Print increment in meters
4	LASTDA		Lewis number, here always 1
4	LASTDA		Prandtl number, here always 1
4	MEFF	TAPE8	Initial Boundary Radius, in meters
4	LASTDA		Factor used to vary eddy viscosity, here always 1
On card 5, all data entered in E1Ø.3			
5	LASTDA		Minimum integration step size, here always .1E-1Ø
5	FLASH	TAPE8	Diffusion step size, FDL
5	LASTDA		Pressure coefficients, here always zero
On card 6, all data entered in E1Ø.3			
6	LASTDA		Pressure at initial value of X, in atmospheres, here always 1
6	MEFF	TAPE8	Temperature at initial boundary in K
6	LASTDA		Ambient air temperature in K, here always 294
6	MEFF	TAPE8	Gas velocity at the initial boundary, in m/s
6	LASTDA		Ambient air velocity in m/s, here always 3.Ø. Should never be set to Ø.
6	LASTDA		Ψ . Here always blank, so program calculates this quantity.
6	LASTDA		Kinetics cut-off temperature in K, here always 2ØØ
7 8 9	LASTDA		Mole fractions of the allowed gaseous species in the ambient air

10			
11	CONCEN	TAPE2	Mole fractions of the allowed gaseous species
12			at the initial boundary

Next in LASTDA come the thermodynamic data on the allowed gaseous species, in JANAF-table format.[6] These are only changed when new data are published. Each species name is entered in A6 format, and all data are then entered in E10.3 format. The ordering of the species in this table determines the order in which LAPP processes the species in all of its transactions. It even specifies which species to associate with the initial number densities which have already been read in from this data set.

Last in LASTDA are the reaction-rate data for the 25 reactions. The reactions may be listed in any order. The data for the C-N-O-H and K reactions have been fairly thoroughly used and checked. At the time this report is written, they are the best available set of reactions and the best available reaction rates for those reactions; but they are not represented here as being the final correct description for the reactions.

The format for each reaction follows:

Column	Item	Format
1-6	Species A	A6
7	+ sign	
8-13	Species B (or M)	A6
14	+ sign (if needed)	
15-20	Blank or M	
21	= sign	
22-27	Species C	A6
28	+ sign (if needed)	
29-34	Species D (or M)	A6
35	+ sign (if needed)	
36-41	Species E (or M)	A6
42-48	Blank	
49-50	Reaction type, 1 to 10 (see below)	I2
51	Rate coefficient type, 1 to 7 (see below)	I1
52-59	A, Pre-exponential factor, cm-molecule-sec units	E8.2
60-63	N, Temperature exponent	F4.1
64-72	B, Activation energy, cal/mole	F9.1

The ten possible reaction types are these:

1	$A + B \rightleftarrows C + D$	
2	$A + B + M \rightleftarrows C + M$	
3	$A + B \rightleftarrows C + D + E$	
4	$A + B \rightleftarrows C$	
5	$A + M \rightleftarrows C + D + M$	
6	$A + B \rightarrow C + D$	
7	$A + B + M \rightarrow C + M$	
8	$A + B \rightarrow C + D + E$	

6. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables, SECOND EDITION," Dow Chemical Company, Midland, MI, July 1970.

9 $A + B \rightarrow C$
10 $A + M \rightarrow C + D + M$

The seven possible rate coefficient types are these:

1 $k = A$

2 $k = AT^{-1}$

3 $k = AT^{-2}$

4 $k = AT^{-\frac{1}{2}}$

5 $k = A \exp (B/RT)$

6 $k = AT^{-N}\exp(B/RT)$

7 $k = AT^{-\frac{3}{2}}$

X. FINAL RESULTS

Some of the pages of the final results of the illustrative calculation are included as Appendix K. The total calculation took 78 CPU seconds on MFZ, all but 14.5 seconds of which was LAPP execution.

MEFF results are followed by BLAKE calculations at the two necessary combinations of temperature and pressure. These are followed by the results of CONCEN, the combined mole fractions at the initial boundary.

Finally come the results of the LAPP calculation. First the input parameters are echoed. Then, at each desired distance from the muzzle, as a function of the distance from the centerline of the flight of the projectile, there are gas temperature, velocity, density, etc. and mole fractions for each of the allowed gaseous consitutents. Included in Appendix K are the prints for the flow from the muzzle (X = Ø meters), for X = 1Ø meters (where one notes a maximum gas temperature of 1Ø79 K), for X = 15.3 meters, and for X= 42 m. The prints at 15.3 meters are the most interesting, for they show that the maximum temperature has risen to 2Ø18 K, indicating that ignition has taken place. If there had been sufficient suppressant to eliminate the flash, one would have seen the temperature rise to 11ØØ K or 12ØØ K and then decline slowly, indicating that the mixture had cooled before ignition could take place.

It was noted earlier that one could set KEY = Ø in the input job stream for MEFF/LAPP (Appendix D), and that then one would have gotten only the centerline temperatures from LAPP. Notice that even then, by 42 meters the centerline temperature has exceeded 2ØØØ K, so that even with a limited print, ignition is unmistakably indicated.

ACKNOWLEDGMENTS

I especially appreciate all of those whose desire to make flash prediction calculations with MEFF and LAPP encouraged me to write this users' guide. They include, but are not limited to, W. Lippincott, P. Baer, T. Coffee, and A. Bracuti.

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1. V. Yousefian, "Muzzle Flash Onset," ARI-RR-236, Aerodyne Research, Inc., Billerica, MA, November 198Ø. Also available as ARBRL-CR-ØØ477, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD February 1982 (AD BØ63 573L).

2. R. R. Mikatarian, C. J. Kau, and H. S. Pergament, "A Fast Computer Program for Nonequilibrium Rocket Plume Predictions," AFRPL-TR-72-94, Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, CA, August 1972.

3. J. Corner, Theory of Interior Ballistics of Guns, John Wiley & Sons, New York (195Ø).

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5. P. G. Baer and J. M. Frankle, "The Simulation of Interior Ballistic Performance of Guns by Digital Computer Program," BRL Report No. 1183, U.S. Army Aberdeen Research and Development Center, Ballistic Research Laboratories, Aberdeen Proving Ground, MD, December 1962 (AD 299 98Ø).

6. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables, SECOND EDITION," Dow Chemical Company, Midland, MI, July 197Ø.

APPENDIX A

BLA3ØA1, INPUT FOR A BLAKE CALCULATION

```
GEK,STMFZ,P6,T12Ø.BLA3ØA1
ACCOUNT,XXXXXX.
ATTACH,TT,BLAKELIBRARY,ID=ELI.
COPY,TT,TAPE7.
RETURN,TT.
REWIND,TAPE7.
ATTACH,B,BLAKE,ID=ELI.
B.
EXIT.
*EOR
TIT,M3ØA1
PRL,CON,2
REJ,N,K2SO4,C,C2,CH,CH2O,HNO3
REJ,C(S),K2SO4$
REJ,KOH$,KO2$,K2O2$
REJ,H2S,S2O,SO2,K$,K2O,K2O2
REJ,KCO$,KSO$,K2O$,K$
REJ,K2CO3$
REJ,K2S$
UNI,ENG
CM2,NC126Ø,27.9,NG,22.42,NQ,46.84,EC,1.49,KS,1.,
ALC,.25,C,.1
GUN,.1,.1,.5
QUIT
```

APPENDIX B

BLAKE CALCULATION

** PROGRAM BLAKE, VERSION 205.11 **

M30A1

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1260	27.900	.018	-1.6916E+08	C 6000 H 7549 O 9901 N 2451
NG	22.420	17.201	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	46.840	78.418	-2.2100E+04	C 1 H 4 O 2 N 4
EC	1.490	.967	-2.5100E+04	C 17 H 20 O 1 N 2
KS	1.000	1.000	-3.4266E+05	K 2 S 1 O 4
ALC	.250	.945	-6.6420E+04	C 2 H 6 O 1
C	.100	1.451	0.	C 1

THE HEAT OF FORMATION IS -384.86 CAL/GRAM = -6.7053E+04 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	14.896
H	32.439
O	28.660
N	23.830
K	.116
S	.058

M30A1

THERE ARE 29 GASEOUS CONSTITUENTS SELECTED

	NAME	BKW CO-VOL	L-J EPS/K	L-J SIGMA	A1	A2	A3	A4	A5	A6	A7	A8	A9
							THERMO CONSTANTS						
1.	CO	390.0	91.7	3.690	5.83775	-.40270	.06491	-.00373	-2.14066	.71717	-.08241	-31130.5	53.1746
2.	H2O	250.0	542.5	2.790	7.60069	.39388	-.10260	.00807	-4.86836	2.30899	-.37689	-62860.1	47.1008
3.	CO2	600.0	195.2	3.941	9.06744	-.40694	.06138	-.00273	-2.70529	.56199	-.04428	-102647.7	60.2574
4.	N2	380.0	71.4	3.798	5.90618	-.39603	.05863	-.00307	-2.41322	.89566	-.11540	-4589.1	51.2455
5.	H2	180.0	59.7	2.827	4.48064	.19824	-.00851	-.00003	-1.97442	1.15151	-.21216	-2116.7	36.2744
6.	NO	386.0	116.7	3.492	5.77838	-.43892	.08202	-.00561	-1.79245	.50895	-.04564	16765.3	57.0969
7.	KOH	0.0	100.0	3.500	7.27052	.40176	-.10705	.00896	-1.70167	.87842	-.16291	-59999.7	68.1294
8.	NH3	476.0	558.3	2.900	13.60629	-.93312	.18185	-.00958	-9.06058	3.51672	-.50840	-22985.7	45.5074
9.	HCN	359.0	344.7	3.339	9.48792	-.37343	.04424	-.00222	-4.59416	1.73907	-.25679	24383.5	53.6459
10.	CH4	528.0	148.6	3.758	20.35251	-1.95871	.26284	-.01397	-14.43248	5.11197	-.67906	-38010.8	38.5449
11.	COS	0.0	130.0	3.500	9.07572	-.47894	.09730	-.00658	-2.27231	.48548	-.04719	-41172.7	66.5255
12.	C2H4	372.0	224.7	4.163	22.63477	-1.64131	.20002	-.00937	-13.78191	4.49325	-.59268	-10548.7	51.3360
13.	C2H2	0.0	100.0	3.500	12.54085	-.16675	.02155	-.00023	-5.90900	2.01409	-.26643	43014.0	54.7220
14.	O2	350.0	106.7	3.467	2.20366	1.12042	-.18485	.01276	2.02364	-1.20737	.22334	-2085.5	59.2300
15.	K	0.0	100.0	3.500	6.09867	-1.44727	.10388	.03850	-3.46738	1.37555	-.18637	16559.0	41.4178
16.	S	0.0	100.0	3.500	1.83331	.19365	.01065	-.00358	.77619	-.26477	.03824	65713.8	47.5476
17.	C2N2	0.0	100.0	3.500	13.82927	-1.13108	.19089	-.01258	-5.06809	1.56648	-.19796	61813.4	70.4037
18.	OH	226.0	100.0	3.500	4.22400	.47240	-.11211	.00942	-1.70189	.97134	-.16944	7437.0	49.0478
19.	KO	0.0	100.0	3.500	4.49837	.11393	.00019	-.00002	.00503	-.02588	.00186	14185.2	67.4039
20.	SO	0.0	100.0	3.500	1.92172	1.33802	-.22714	.01363	2.24044	-1.13902	.18518	-219.7	63.6970
21.	S2	0.0	100.0	3.500	4.48800	.03544	-.00050	.00003	.02430	-.11854	.01769	27643.9	64.5607
22.	HS	0.0	100.0	3.500	6.12907	-.41325	.06726	-.00371	-2.95581	1.32672	-.19604	30547.3	51.9361
23.	CH3	525.0	100.0	3.500	13.82287	-.74765	.05695	-.00032	-9.14376	3.65133	-.54025	23004.1	46.4265
24.	H	13.4	100.0	3.500	2.49993	.00000	-.00000	.00000	.00000	-.00000	.00600	50621.8	33.4041
25.	O	212.8	100.0	3.500	2.97972	-.25641	.05953	-.00389	-.43119	.19753	-.02943	57760.7	44.3789
26.	CHO	700.0	100.0	3.500	10.04357	-1.09647	.20969	-.01480	-4.57561	1.36019	-.14753	955.9	59.4686
27.	CH2	525.0	100.0	3.500	11.42150	-1.32276	.21610	-.01403	-7.38097	3.01187	-.44496	83047.1	47.9048
28.	CN	0.0	100.0	3.500	2.71179	.54169	.09568	-.02040	1.50282	-1.01851	.20537	101465.0	58.3631
29.	K2	0.0	100.0	3.500	4.50198	.24737	.00004	.00000	-.00245	-.00020	-.00023	27675.0	70.3214

THE FLOOR IS AT 14

** PROGRAM BLAKE, VERSION 205.11 **

18 AUG, 1983 PAGE 3

M30A1

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		1)	2)	3)
N2	GAS	1.17839E+01	1.17756E+01	1.17633E+01
CO	GAS	1.16845E+01	1.17189E+01	1.17434E+01
H2O	GAS	1.04224E+01	1.04928E+01	1.05490E+01
H2	GAS	5.49904E+00	5.42160E+00	5.33950E+00
CO2	GAS	3.04189E+00	2.99399E+00	2.95515E+00
KOH	GAS	1.02155E-01	1.06154E-01	1.08132E-01
COS	GAS	1.24913E-02	1.97122E-02	2.57452E-02
NH3	GAS	9.60859E-03	2.35990E-02	4.35205E-02
NO	GAS	6.45435E-03	4.35300E-03	3.34043E-03
HCN	GAS	2.72481E-03	7.11492E-03	1.39539E-02
O2	GAS	2.42410E-04	1.03891E-04	5.79830E-05
CH4	GAS	8.74142E-05	4.65937E-04	1.40821E-03
C2H2	GAS	1.10729E-06	6.86994E-06	2.40198E-05
C2H4	GAS	2.48644E-08	3.29884E-07	1.86232E-06
K	GAS	1.24966E-02	8.52656E-03	6.57183E-03
S	GAS	1.96564E-03	1.24340E-03	8.54751E-04
C2N2	GAS	2.72369E-08	1.91412E-07	7.57681E-07
OH	GAS	3.90690E-02	2.46999E-02	1.77802E-02
KO	GAS	1.14157E-04	8.08104E-05	6.38757E-05
SO	GAS	1.37149E-02	8.67324E-03	5.96825E-03
S2	GAS	1.81570E-03	1.72835E-03	1.48727E-03
HS	GAS	2.55860E-02	2.43007E-02	2.18473E-02
CH3	GAS	2.38187E-05	8.77368E-05	2.09539E-04
H	GAS	6.42166E-02	4.01198E-02	2.86234E-02
O	GAS	2.96179E-04	1.26138E-04	5.99457E-05
CHO	GAS	1.83960E-03	2.95975E-03	4.09603E-03
CH2	GAS	6.12020E-07	1.52314E-05	2.80760E-06
CN	GAS	4.36160E-06	7.55025E-06	1.11839E-05
K2	GAS	4.83636E-06	5.66071E-06	6.34867E-06
TOTAL GAS (MOLES/KG)		42.7266	42.6770	42.6341

M30A1

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

	RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT GAS	CO-VOL CC/G	FROZEN GAMMA	CP(FR) J/MOL-K	B(T) CC	C(T) CM**6	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1)	.1000	2992.	119.22	1062.9	23.405	1.084	1.2380	43.77	26.09	555.	10.000	9.57	-418.2	-1610.3	1.3738	1.1216
2)	.2000	3003.	269.13	1065.3	23.432	1.041	1.2412	44.20	26.08	555.	5.000	9.29	-264.6	-1610.2	1.5338	1.2629
3)	.3000	3010.	455.81	1066.9	23.455	.993	1.2471	44.73	26.06	555.	3.333	9.12	-90.9	-1610.2	1.6953	1.4241

	RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT GAS	CO-VOL CU IN	FROZEN GAMMA	CP(FR) CAL/M-K	B(T) CU IN	C(T) IN**6	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1)	.1000	2992.	17291.	355609.	23.405	30.01	1.2380	10.46	1.592	2.07	276.799	2.29	-99.9	-384.9	1.3738	1.1216
2)	.2000	3003.	39034.	356461.	23.432	28.81	1.2412	10.56	1.591	2.07	138.399	2.22	-63.2	-384.9	1.5338	1.2629
3)	.3000	3010.	66110.	356933.	23.455	27.48	1.2471	10.69	1.590	2.06	92.266	2.18	-21.7	-384.9	1.6953	1.4241

APPENDIX C

IBHVG CALCULATION

GUN TYPE: 155-MM HOWITZER
CHAMBER VOLUME: 1200.00 CU IN
GROOVE DIAMETER: 6.200 IN
GROOVE/LAND RATIO: 1.660
TWIST: ONE TURN IN 20.0 CALIBERS
PRESSURE GRADIENT: LAGRANGIAN
PROJECTILE: M483A1

BORE LENGTH: 200.0 IN
TIME STEP: .100 MS
LAND DIAMETER: 6.100 IN
BORE AREA: 29.828 SQ IN
EXPANSION RATIO: 6.0
EROSIVE COEFF: .0000500
PROJ WT: 102.200 LB

ENGRAVING & FRICTIONAL RESISTANCE [KPSI] VS. TRAVEL [IN]:

TRAVEL:	0.00	.40	1.00	1.55	2.05	4.50	200.00
RESISTANCE:	.25	3.35	4.95	3.63	3.25	2.80	1.50

PROPELLANT	BLK POWDR	M30A1	NC TUBE
WEIGHT [LB]	.315	26.150	.500
IMPETUS [FT-LB/LB]	96000.	356461.	180000.
FLAME TEMP [K]	2000.	3003.	1553.
ALPHA	0.0000	.7000	0.0000
BETA	50.000000	.003950	30.000000
GAMMA	1.250	1.241	1.250
COVOL [CU IN/LB]	30.000	28.810	30.000
DENS [LB/CU IN]	.06000	.05717	.03400
GRAIN TYPE	CORD	7-PERF	SHEET
GRAIN LEN [IN]	.2000	.9481	28.0000
GRAIN WIDTH [IN]	-------	-------	1.5000
GRAIN DIAM [IN]	.1000	.4173	-------
PERF DIAM [IN]	-------	.0338	-------
GRAIN THICK [IN]	-------	-------	.1250
INNER WEB [IN]	-------	.0790	-------
OUTER WEB [IN]	-------	.0790	-------
IGNITION CODE	0	0	0
THRESHOLD VALUE	0.00000	0.00000	0.00000

STDM203, A STANDARD M203 CHARGE IN A 155-MM HOWITZER

CONDITIONS AT:	MAX PR	MUZZLE	PROP 1 BURNT	PROP 2 BURNT	PROP 3 BURNT
TIME [MS]	6.65	13.69	1.00	11.20	2.10
BR PRES [KPSI]	47.77	11.48	3.01	19.96	9.04
MN PRES [KPSI]	46.02	11.10	2.91	19.26	8.81
BS PRES [KPSI]	42.52	10.34	2.72	17.88	8.35
MEAN TEMP [K]	2622.	1860.	2266.	2088.	2530.
TRAVEL [IN]	23.9	200.0	.0	124.4	.4
VEL [FPS]	1104.	2650.	9.	2377.	48.
ACCEL [G'S]	11615.	2530.	644.	4593.	1524.
FR BRNT PROP 1	1.000	1.000	1.000	1.000	1.000
FR BRNT PROP 2	.571	1.000	.010	1.000	.043
FR BRNT PROP 3	1.000	1.000	.502	1.000	1.000

APPENDIX D

FLASH, THE JCL AND INPUT DATA FOR MEFF, MTOB, BLAKE, CONCEN, AND LAPP

```
GEK,STMFZ,P1,T3ØØ.FLASH
ACCOUNT,XXXXXXX.
BEGIN,GETMFA,FILE,LF=A,PF=MEFF,UN=GEK.CREATES TAPE9
MAP,OFF.
FTN,I=A,L=Ø,R=Ø,T.
LGO.
REWIND,TAPE9.
BEGIN,GETMFA,FILE,LF=E,PF=MTOB,UN=GEK.
BEGIN,GETMFA,FILE,LF=TAPE4,PF=BOIL,UN=GEK.BLAKE BOILERPLATE
FTN,B=LGO3,I=E,L=Ø,R=Ø,T.
LGO3.
REWIND,OUTPUT.
COPY,OUTPUT,TAPE8.
REWIND,TAPE8.FILE OF BLAKE, CONCEN, AND LAPP DATA
ATTACH,TT,BLAKELIBRARY,ID=ELI.
COPY,TT,TAPE7.
RETURN,TT.
REWIND,TAPE7.
ATTACH,B,BLAKE,ID=ELI.
B,TAPE8.
REWIND,OUTPUT.
REWIND,TAPE1.
COPY,OUTPUT,TAPE1.
REWIND,TAPE1. INPUT FOR CONCEN
BEGIN,GETMFA,FILE,LF=C,PF=CONCEN,UN=GEK.
FTN,B=LGO1,I=C,L=Ø,R=Ø,T.
LGO1.
REWIND,TAPE2.
BEGIN,GETMFA,FILE,LF=TAPE3,PF=LASTDA,UN=GEK.
REWIND,TAPE3.
BEGIN,GETMFA,FILE,LF=D,PF=LAPP,UN=GEK.
FTN,B=LGO2,I=D,L=Ø,R=Ø,T.
LGO2.
EXIT.
 155-MM HOWITZER WITH M2Ø3 CHARGE
8Ø7.7,.Ø19664,5.Ø8,12.23,46.36,.Ø19244,1.241,23.432,186Ø.,.ØØ1Ø41
4,.ØØ1,.Ø1
5Ø.,5.Ø,Ø.2Ø,1
```

APPENDIX E
MEFF PROGRAM LISTING

```
      PROGRAM MEFF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9)
C
C MAIN: MUZZLE FLASH
C
C MUZZLE PROPERTIES VS TIME
C
C TYPE DATA CARDS USING NAMELIST FORMAT
C
C     TITLE CARD FIRST
C
C      *PHYSIC*
C             VØ=MUZZLE VELOCITY(M/SEC)
C             L=BORE LENGTH(M)
C             MP=MASS OF PROPELLANT
C             W=MASS OF PROJECTILE(KG)
C             A=CROSS SECTIONAL AREA OF BORE(M**2)
C             GAM=RATIO SPECIFIC HEATS PROPELLANT GAS
C             MBAR=MEAN MOL WEIGHT PROPELLANT
C             TF=FLAME TEMPERATURE(K)
C             TA=AVERAGE BARREL GAS TEMPERATURE(K)
C             CVO=CHAMBER VOLUME(M**3)
C             ETA=COVOLUME FOR VAN DER WAAL'S EQ. STATE(M**3/KG)
C      *MATH*
C             M=NUMBER OF ITERATIONS BETWEEN STORED VALUES
C             DELTAU=STEP SIZE
C             DLTAUØ=INITIAL CONDITION STEP AWAY FROM TAU=Ø
C
      REAL MP,L,MBAR,LAMM,MØ,MACHNO,MR,MNP2
      COMMON/WORKA/LAMM,GAM,EPS,MØ,BØ,CØ,DØ,KPMAX
      COMMON/WORKB/THETA(5ØØ),Z(5ØØ),H1(5ØØ),H1P(5ØØ),THETAP(5ØØ),
     1 TTAU(5ØØ),FEJECT(5ØØ)
      COMMON/WORKC/TEFF,ETA,A,L,MP,VØ,ALMP,R
      COMMON/WORKD/PE(5Ø),UE(5Ø),TE(5Ø),RHOE(5Ø),TIME(5Ø),
     1 TEMP(5Ø),FKP(5Ø),CO2(5Ø),CO(5Ø),H2O(5Ø),H2(5Ø)
      DIMENSION TITLE(2Ø)
      NAMELIST/PHYSIC/VØ,L,MP,W,A,GAM,MBAR,TF,TA,ETA,CVO
      NAMELIST/MATH/M,DELTAU,DLTAUØ
      DATA IREAD,IWRITE/5,6/
      DATA IMAX/5ØØ/,IZTHET/Ø/,PI/3.141592654/
C
C READ IN DATA
C
      READ(IREAD,1111)TITLE
 1111 FORMAT(2ØA4)
      WRITE(9,1111)TITLE
 1ØØØ FORMAT(1H1,2ØA4)
      READ(IREAD,*)VØ,CVO,L,MP,W,A,GAM,MBAR,TA,ETA
C     CALL NMLST('PHYSIC',Ø,5,VØ,L,MP,W,A,GAM,MBAR,TF,TA,ETA,CVO)
      READ(IREAD,*)M,DELTAU,DLTAUØ
C     CALL NMLST('MATH  ',Ø,5,M,DELTAU,DLTAUØ)
C
C READ MAX DIST, PRINT STEP, DIFFUSION STEP SIZE, AND KEY; ALL FOR LAPP.
C KEY=1 FOR ALL LAPP PRINTS, =Ø FOR CENTERLINE ONLY.
C
      READ(IREAD,*)XMAX,PRNT,FDL,KEY
```

```
C
      CALBER = 1000. * SQRT( 4.*A/3.141593 )
C
      IF(TF.EQ.0.0) GO TO 1
      WRITE(IWRITE,1000) TITLE
      WRITE(IWRITE,1010) V0,L,MP,W,CALBER,A,GAM,MBAR,TF,ETA,
     1CVO
 1010 FORMAT('0',' MUZZLE VELOCITY V0 =',G10.4,' M/SEC'/
     1' ',' BORE LENGTH L =',G10.4,' METERS'/
     2' ',' PROPELLANT MASS MP =',G10.4,' KG'/
     3' ',' PROJECTILE MASS W =',G10.4,' KG'/
     4' ',' GUN CALIBER  CALBER =',G10.4,' MM'/
     5' ',' BARREL CROSS SECTIONAL AREA A =',G10.4,' M**2'/
     6' ',' SPECIFIC HEAT RATIO OF PROPELLANT GAS  GAM =',G10.4/
     7' ',' MEAN MOLECULAR WEIGHT OF PROPELLANT GAS  MBAR =',G10.4,
     8 /
     9' ',' FLAME TEMPERATURE  TF =',G10.4,' DEG K'/
     1' ',' COVOLUME ETA =',G10.4,' M**3/KG'/
     2' ',' CHAMBER VOLUME CVO =',G10.4,' M**3'/)
      WRITE(6,6001)
      GO TO 6000
    1 WRITE(IWRITE,1000) TITLE
      WRITE(IWRITE,1110) V0,L,MP,W,CALBER,A,GAM,MBAR,TA,ETA,
     1 CVO
 1110 FORMAT('0',' MUZZLE VELOCITY V0 =',G10.4,' M/SEC'/
     1' ',' BORE LENGTH L =',G10.4,' METERS'/
     2' ',' PROPELLANT MASS MP =',G10.4,' KG'/
     3' ',' PROJECTILE MASS W =',G10.4,' KG'/
     4' ',' GUN CALIBER  CALBER =',G10.4,' MM'/
     5' ',' BARREL CROSS SECTIONAL AREA A =',G10.4,' M**2'/
     6' ',' SPECIFIC HEAT RATIO OF PROPELLANT GAS  GAM =',G10.4/
     7' ',' MEAN MOLECULAR WEIGHT OF PROPELLANT GAS  MBAR =',G10.4,
     8 /
     9' ',' AVERAGE BARREL GAS TEMPERATURE  TA =',G10.4,' DEG K'/
     1' ',' COVOLUME ETA =',G10.4,' M**3/KG'/
     2' ',' CHAMBER VOLUME CVO =',G10.4,' M**3'/)
      WRITE(6,6001)
 6000 CONTINUE
C
C CALCULATED PARAMETERS
C
      L=L+CVO/A
      ALMP = A*L/MP
      LAMM=MP/W
      R=8317./MBAR
      TEFF = TF - .5*(GAM-1.)*V0*V0*(.3333+1./LAMM)/R
      IF(TA.NE.0.0)TEFF=TA
      EPS=ETA/(ALMP-ETA)
      M0=V0/SQRT(GAM*R*TEFF)
C
C
C INITIAL CONDITIONS: THET0
C
      C=1.+EPS
      G10=C+LAMM/(3.*GAM)
```

```
      G1ØP=G1Ø-LAMM*(C/MØ+.5)/GAM
C
      J = Ø
      YOLD = (2.-MØ+C)/(MØ+C)
      EXP = 2./(GAM+1.)
   2Ø J = J + 1
      IF(J.GE.15) GO TO 2Ø
      DENOM = MØ + 1. + EPS + (MØ-1.-EPS)/YOLD
      YNEW = (EPS + (2.*G1Ø/DENOM)**EXP) / G1Ø
C
      IF(ABS(YNEW-YOLD).LE..ØØØØ1) GO TO 3Ø
      YOLD = YNEW
      GO TO 2Ø
C
   3Ø THETØ = YNEW
C
C
C INITIAL CONDITIONS: THETØP
C
      ALPHA=.5*(GAM+1.)/(1.-EPS/(THETØ*G1Ø))
      BETA=-1.*THETØ*(MØ+C)/(MØ-C)
      BPRIME=-1.+LAMM/(GAM*MØ*MØ)
      CPRIME=.5*(1.-GAM)-GAM*EPS
      DELTA=(BPRIME*(1.+THETØ)+CPRIME*(THETØ-1.)/MØ)/(1.-C/MØ)
      THETØP =THETØ*((1.+THETØ)*(1.-G1ØP/G1Ø)+DELTA+
     1G1ØP*(1.-ALPHA)*(BETA-1.)/G1Ø)/(2.+ALPHA*(BETA-1.))
C
C
C SUBROUTINE ZTHETA INTEGRATES  DIFFERENTIAL EQ. FOR  THETA
C ZTHETA CALLS RUNGE-KUTTA SCHEME SUBROUTINES GILL AND GILL1
C ZTHETA CALLS DERIV TO CALCULATE DERIVATIVES OF Z AND THETA
C
      CALL ZTHETA(DELTAU,DLTAUØ,THETØ,THETØP,IMAX,M,I,G1Ø,EJECTO)
C
C PRINT MUZZLE PROPERTIES
C
      DO 6Ø K=1,I
      T=TTAU(K) * L/VØ * 1ØØØ.
      RHO2=EPS/(ETA*H1(K))
      V2=SQRT(GAM*R*TEFF)*H1(K)/(H1(K)-EPS)**(.5*(GAM+1.))
      T2=TEFF*(H1(K)-EPS)**(1.-GAM)
      P2=R*T2/(1./RHO2-ETA)
      P2ATM = P2 / 1Ø1325.
      SONICV = SQRT( GAM*R*T2 )
      MACHNO = V2 / SONICV
      FEJECT(K) =FEJECT(K)/ MØ / (1.-ETA*MP/(A*L))
      IF(MACHNO.LT.1.Ø)GO TO 1ØØ1
      ZSQ=.476*GAM*P2ATM
      ZSQ1=SQRT(ZSQ)
      XM2=(.4*ZSQ)**(GAM-1.)*(GAM+1.)/((GAM-1.)**GAM)
      DO 2ØØØ J=1,5Ø
      AB=1./(GAM-1.)
      ABC=AB*GAM
      ABCD=(2.+(GAM-1.)*XM2)
      ABCDE=2.*GAM*XM2-(GAM-1.)
```

```
      XFMP=-.49*GAM**2*(1./(GAM+1.))**AB*(ABCD**AB-2.*ABCD**ABC/ABCDE)/
     1ABCDE
      XFM=ZSQ-.49*GAM*(1./(GAM+1.))**AB*ABCD**ABC/ABCDE
C     WRITE(1,2001)XFM,XM2
      IF(ABS(XFM).LT..001) GO TO 2002
      XM2=XM2-XFM/XFMP
      IF(J.EQ.50)STOP 10
 2000 CONTINUE
 2002 XM1=SQRT(XM2)
      PM0=R*TEFF*(1.0-LAMM/3.0)/(ALMP-ETA)
      PM0=PM0/101325.
      TM0=TEFF*(1.0-(GAM-1.0)*LAMM/(GAM*3.0))
      GAMP1=GAM+1.0
      GAMM1=GAM-1.0
      AXX=GAMM1/GAM
      MR=(GAMP1*P2ATM**AXX-2.0)/GAMM1
      MR=SQRT(MR)
      TR=T2*GAMP1/(2.0+GAMM1*MR**2)
      UR=SQRT(GAM*R*TR)*MR
      TN1=GAMP1/(2.0+GAMM1*XM1**2)
      TN2=1.0+2.0*GAMM1*(GAM*XM2+1.0)*(XM2-1.0)/(XM2*GAMP1**2)
      TN=TN1*TN2*T2
      MNP2=(2.0+GAMM1*XM2)/(2.0*GAM*XM2-GAMM1)
      UN=SQRT(MNP2*R*TN*GAM)
      EPSD=0.69*SQRT(GAM*P2ATM)
      XXY=GAMP1/(2.0*GAMM1)
      XXYY=(GAMP1/(2.0+GAMM1*XM2))**XXY
      TETTA=0.96*EPSD**2*XM1*XXYY
      UB=(1.0-TETTA)*UR+TETTA*UN
      TB1=(1.0-TETTA)*TETTA*GAMM1/2.0
      TB2=MR**2*(1.0-(UN/UR)**2)*TR
      TB=(1.0-TETTA)*TR+TETTA*TN+TB1*TB2
      PR=1.0
      UMS=SQRT(GAM*R*T2)
      AB=P2ATM*(TB/T2)*(UMS/UB)*A
      RB=SQRT(AB/PI)
      WRITE(6,5000)
 5000 FORMAT(32X,48HMUZZLE GAS PROPERTIES WHEN PROJECTILE IS EJECTED,/)
      WRITE(6,6001)
      WRITE(6,5001)PM0
 5001 FORMAT(40X,9HPRESSURE=,2X,F7.2,4H ATM)
      WRITE(6,5002)TM0
 5002 FORMAT(40X,12HTEMPERATURE=,2X,F7.1,2H K)
      WRITE(6,5003)V0
 5003 FORMAT(40X,9HVELOCITY=,2X,F7.1,6H M/SEC)
      WRITE(6,6001)
 6001 FORMAT(2X,///)
      WRITE(6,5004)
 5004 FORMAT(32X,56HMUZZLE GAS PROPERTIES WHEN MUZZLE VELOCITY BECOMES S
     1ONIC,/)
      WRITE(6,6001)
      WRITE(6,5001)P2ATM
      WRITE(6,5002)T2
      WRITE(6,5003)UMS
      FEJ=FEJECT(K)
```

```
      WRITE(6,5ØØ5)FEJ
 5ØØ5 FORMAT(4ØX,31HFRACTION OF EJECTED PROPELLANT=,2X,F6.4)
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ6)
 5ØØ6 FORMAT(32X,69HFLOW CONDITIONS AT REFLECTED SHOCK WHEN MUZZLE VELOC
     1ITY BECOMES SONIC,/)
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ1)PR
      WRITE(6,5ØØ2)TR
      WRITE(6,5ØØ3)UR
      ALPH1=1.Ø-TETTA
      WRITE(6,5ØØ7)ALPH1
 5ØØ7 FORMAT(4ØX,41HFRACTION OF GAS ENTERING REFLECTED SHOCK=,2X,F6.4)
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ8)
 5ØØ8 FORMAT(32X,66HFLOW CONDITIONS AT NORMAL SHOCK WHEN MUZZLE VELOCITY
     1 BECOMES SONIC,/)
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ1)PR
      WRITE(6,5ØØ2)TN
      WRITE(6,5ØØ3)UN
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ9)
 5ØØ9 FORMAT(32X,76HFLOW CONDITIONS AT MIXING REGION BOUNDARY WHEN MUZZL
     1E VELOCITY BECOMES SONIC,/)
      WRITE(6,6ØØ1)
      WRITE(6,5ØØ1)PR
      WRITE(6,5ØØ2)TB
      WRITE(6,5ØØ3)UB
      WRITE(6,5Ø1Ø)RB
 5Ø1Ø FORMAT(4ØX,17HBOUNDARY RADIUS =,2X,F6.3,' M',////)
C
      WRITE(9,5Ø11)TN,TMØ,TB,PMØ,UB,ALPH1,RB,XMAX,PRNT,FDL,KEY
 5Ø11 FORMAT(1ØF8.3,I1)
C THUS IS DATA PASSED ON TO MTOB, BLAKE, CONCEN, AND LAPP
C
 5555 FORMAT(1H ,"MACH NO IS .GE. 1")
      IF(MACHNO.GE.1.Ø)WRITE(6,5555)
      IF(MACHNO.GE.1.Ø)STOP
C
 1ØØ1 CONTINUE
C
      WRITE(IWRITE,1Ø9Ø) T,RHO2,V2,P2,P2ATM,T2,SONICV,MACHNO,FEJECT(K)
 1Ø9Ø FORMAT(' ',1P9G13.4)
C
   6Ø CONTINUE
      IF(I.GT.1)STOP
C
C
C SUBROUTINE RATEAU CALCULATES THE MUZZLE PROPERTIES AFTER
C THE RAREFRACTION WAVE HITS THE BREECH
C
      WRITE(IWRITE,11ØØ)
 11ØØ FORMAT('Ø RAREFRACTION WAVE HAS HIT THE BREECH'//)
      T = TTAU(I)*L/VØ*1ØØØ.
```

```
      T2 = TEFF*(H1(I)-EPS)**(1.-GAM)
      EJECTO = EJECTO/MØ/(1.-ETA*MP/(A*L))
      CALL RATEAU(T,T2,EJECTO,I,JJ)
C
C PLANE A
C
      WRITE(IWRITE,211Ø)
 211Ø FORMAT('1',T45,'PLANE A FLOW PROPERTIES'//' TIME',T1Ø,
     1 'DENSITY',T2Ø,'TEMP',T3Ø,'VELOCITY',T43,'XI/D',T5Ø,'SHOCK',
     2 T6Ø,'PLANE A',T7Ø,'CO2',T8Ø,'CO',T9Ø,'H2O',T1ØØ,'H2'/
     3'  MSEC',T11,'KG/M3',T21,'DEG K',T31,'M/SEC',T5Ø,'LENGTH',
     4 T6Ø,'DIAMETER',T7Ø,'MOL/M3',T8Ø,'MOL/M3',T9Ø,'MOL/M3',
     5 T1ØØ,'MOL/M3'/)
C
      DO 7Ø I=1,JJ
      PØ = PE(I)*((GAM+1.)*.5)**(GAM/(GAM-1.))
      XID = .69*SQRT(GAM*PE(I))
      XID = XID/(1. + .197*PHI**.65)
      SHOCKL = 1.25*XID
      HAREA = A*SQRT(.5*(GAM-1.))*(2./(GAM+1.))**((GAM+1.)*.5/
     1 (GAM-1.))
      HAREA = HAREA/SQRT(1.-PØ**((1.-GAM)/GAM))
      HAREA = HAREA*PØ**(1./GAM)
      HDIA = SQRT(HAREA/A)
      RHOA = RHOE(I)/PE(I)**(1./GAM)
      TA = TE(I)/PE(I)**((GAM-1.)/GAM)
      UA = UE(I)*(A/HAREA)*PE(I)**(1./GAM)
      WRITE(IWRITE,112Ø) TIME(I),RHOA,TA,UA,XID,SHOCKL,HDIA,
     1 CO2(I),CO(I),H2O(I),H2(I)
 112Ø FORMAT(1P11G1Ø.3)
   7Ø CONTINUE
C
C ISENTROPIC REGION AND MACH DISC
C
      WRITE(IWRITE,113Ø)
 113Ø FORMAT('1',T45,'ISENTROPIC REGION FLOW FIELD'//
     1T5,'TIME',T2Ø,'R/D',T35,'MACH NO.',T5Ø,'RHO',T65,
     2 'PRESSURE',T8Ø,'TEMPERATURE',T95,'VELOOCITY'/
     3T6,'MSEC',T5Ø,'KG/M3',T66,'ATM',T81,'DEG K',T96,'M/SEC'/)
C
      DO 9Ø KK=5,JJ,5
      XID = .69*SQRT(GAM*PE(KK))
      XID = XID/(1. + .197*PHI**.65)
      STEP = .1*XID
      ROVERD = .69*SQRT(2.*GAM) - STEP
   8Ø ROVERD = ROVERD + STEP
      IF(ROVERD.GE.XID) ROVERD = XID
      CALL MACHN(ROVERD,FMACH,PHI,GAM,XID)
      RHOI = RHOE(KK)*((1.+GAM)/(2.+(GAM-1.)*FMACH*FMACH))**
     1(1./(GAM-1.))
      RATIO = RHOI/RHOE(KK)
      PI = PE(KK)*(RATIO)**GAM
      TI = TE(KK)*(RATIO)**(GAM-1.)
      UI = UE(KK)*FMACH*(RATIO)**(.5*(GAM-1.))
      WRITE(IWRITE,114Ø) TIME(KK),ROVERD,FMACH,RHOI,PI,TI,UI
```

```
 1140 FORMAT(1P7G15.4)
      IF(ROVERD.LT.XID) GO TO 80
      FMACHS = FMACH*FMACH
      FMACH2 = (1. + .5*(GAM-1.)*FMACHS)/(GAM*FMACHS-.5*(GAM-1.))
      FMACH2 = SQRT(FMACH2)
      RHOMD2 = RHOI*(GAM+1.)*FMACHS/((GAM-1.)*FMACHS+2.)
      PMD2 = 1.
      TMD2 = TE(KK)*(2.*GAM*FMACHS-GAM+1.)/(GAM+1.)/FMACHS
      UMD2 = RHOI/RHOMD2*UI
      WRITE(IWRITE,1150) TIME(KK),ROVERD,FMACH2,RHOMD2,PMD2,TMD2,UMD2
 1150 FORMAT(1P7G15.4//)
   90 CONTINUE
C
      WRITE(IWRITE,1160)
 1160 FORMAT('0','  THIS IS THE END OF THE PROGRAM''S OUTPUT')
C
      STOP
      END
C
C
C
      SUBROUTINE ZTHETA(DELTAU,DLTAU0,THET0,THET0P,IMAX,M,I,
     1 G10,EJECTO)
C
C ZTHETA DETERMINES Z(TAU) AND THETA(TAU) USING
C RUNGE-KUTTA INTEGRATION SCHEME
C     IMAX=DIMENSION OF Z IN MAIN PROGRAM
C     I=HIGHEST SUBSCRIPT FOR WHICH VALUES STORED IN Z
C     M=NUMBER OF ITERATIONS BETWEEN STORRED VALUES
      DOUBLE Y(20),DERY(20),Q(20),G1,G1P
      REAL M0,LAMM
C     EXTERNAL DERIV
      COMMON /G/ Q,A(4),B(4),C(4)
      COMMON/WORKB/THETA(500),Z(500),H1(500),H1P(500),THETAP(500),
     1 TTAU(500) ,FEJECT(500)
      COMMON/WORKA/LAMM,GAM,EPS,M0,B0,C0,D0,KPMAX
C
C INITIAL CONDITIONS
C
      THETA(1)=THET0+THET0P*DLTAU0
      TAU=DLTAU0
      TTAU(1) = DLTAU0
      Y(1)=THETA(1)
      DERY(1) = THET0P
      EXPON = -.5*(GAM+1.)
C
C DERIV DETERMINES DY/DX AND THE VALUES OF G1 AND G1P
C
C     CALL DDERIV
      NSUB=1
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
C     CALL DERIV(TAU,Y,DERY,G1,G1P)
      NSUB=2
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
      Z(1)= Y(2)
```

```
      THETAP(1) = DERY(1)
      H1(1)=Y(1)*G1
      H1P(1)=DERY(1)*G1+Y(1)*G1P
      FEJECT(1) = .5*(((THETØ*G1Ø-EPS)**EXPON) +((Y(1)*G1-EPS)
     1**EXPON))*DLTAUØ
      EJECT = FEJECT(1)
      G1OLD = G1
C
C GILL INITIALIZES RUNGE - KUTTA ROUTINE GILL1
C
C     CALL GILL(1,Q,DERIV)
      CALL GILL(1)
      I=1
   1Ø I=I+1
      IF(I.GE.IMAX) GO TO 5Ø
C
C GILL1 INTEGRATES ONE STEP REPLACING TAU AND Y WITH NEW VALUES
C
      Y1OLD = THETA(I-1)
      Y2OLD=Z(I-1)
C
      DO 3Ø J=1,M
      CALL GILL1(DELTAU,TAU,Y,DERY)
C
C STOPING CONDITION: Z(TAUØ)=Ø ; LINEAR INTERPOLATION DETERMINES
C TAUØ & THETA(TAUØ)
C
      IF(Y(2).GE.Ø.Ø) GO TO 2Ø
      R=Y2OLD/Y(2)
      TAUØ=TAU-DELTAU/(1.-R)
      TTAU(I) = TAUØ
      Y(2) = Ø.
      Z(I) = Y(2)
C
      SLOPE = (Y(1)-Y1OLD)/DELTAU
      Y(1) = SLOPE*(TAUØ-TAU) + Y(1)
      THETA(I)=Y(1)
C
C     CALL DERIV(TAUØ,Y,DERY,G1,G1P)
      NSUB=2
      CALL DERIV(TAUØ,Y,DERY,G1,G1P,NSUB)
      THETAP(I) = DERY(1)
      H1(I)=Y(1)*G1
      H1P(I)=DERY(1)*G1+Y(1)*G1P
      FEJECT(I) = EJECT+.5*(((Y1OLD*G1OLD-EPS)**EXPON)+
     1((Y(1)*G1-EPS)**EXPON))*DELTAU
      EJECTO = .5*((Y(1)*G1-EPS)**EXPON)*DELTAU
      RETURN
C  2Ø CALL DERIV(TAU,Y,DERY,G1,G1P)
   2Ø NSUB=2
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
      EJECT = EJECT +.5*(((Y1OLD*G1OLD-EPS)**EXPON)+
     1((Y(1)*G1-EPS)**EXPON))*DELTAU
      G1OLD = G1
      Y1OLD = Y(1)
```

```
      Y2OLD = Y(2)
   3Ø CONTINUE
C
      THETA(I)=Y(1)
      TTAU(I) = TAU
      Z(I) =Y(2)
      THETAP(I) = DERY(1)
      H1(I)=Y(1)*G1
      H1P(I)=DERY(1)*G1+Y(1)*G1P
      FEJECT(I) = EJECT
C
      GO TO 1Ø
C
   5Ø RETURN
      END
      SUBROUTINE DERIV(TAU,Y,DERY,G1,G1P,NSUB)
C     SUBROUTINE DDERIV
C DERIV CALCULATES DY/DX     Y(1)=THETA     DERY(1)=THETP
C                              Y(2)=Z          DERY(2)=ZP
      DOUBLE Y(2),DERY(2),G1,G1P,B,C,F,F1,F2
      REAL MØ,LAMM
      COMMON /WORKA/LAMM,GAM,EPS,MØ,BØ,CØ,DØ,KPMAX
C
      IF(NSUB.NE.1) GO TO 3Ø
C
C CONSTANTS
      AA=LAMM/(GAM*MØ*MØ)
      A1=AA/(2.-GAM)
      A2=1.+EPS-LAMM/(6.*GAM)+AA/(GAM-1.)
      A3=A1/(1.-GAM)
      A4=LAMM/(2.*GAM)
      A8=1.+EPS-AA*.5
      A9=-1.*EPS*(GAM+1.)*.5
      A1Ø=(1.-GAM)*A1*.5
C
      BB = GAM - 1.
      BBB = 2. - GAM
      B1 = 1. + AA/BB - 2./(BB*MØ)*(1.+AA/(3.*BB))
      B2 = 2./(BB*MØ)
      B3 = 1. - AA/2.
      B4 = -.5*AA*BB/BBB
      B5 = -.5*EPS*BB
      B6 = (GAM + 1. )*AA/(6.*BB*BBB)
      B7 = -1.*AA/BBB
      B8 = AA/(BB*BBB)
C
      RETURN
C
C     CALL DERIV(TAU,Y,DERY,G1,G1P)
   3Ø CONTINUE
C EQUATIONS
C
      F=1.+TAU
C
      F1 = B3 + (B4+B5*TAU)/F + B6/F**BB
```

```
      F2 = 1. + B7/F + B8/F**BB
      Y(2) = F * (B1 + B2/F**(.5*BB) * F1)/F2
C
      B=1./F-A1/(F*F)+A1/F**GAM
      C=F**(.5*(1.-GAM))*(A8+A9*TAU/F+A1Ø/F+A1*.5/F**(GAM-1.))
      DERY(2)=B*Y(2)-C/MØ
C
      G1=A1+A2*F+A3*F**(2.-GAM)+A4*Y(2)*Y(2)/F
      G1P=A2+(2.-GAM)*A3*F**(1.-GAM)+A4*(-1.*Y(2)*Y(2)/(F*F)+
     12.*Y(2)*DERY(2)/F)
      IF(TAU.EQ.Ø.) GO TO 6Ø
      FACT=Y(1)*G1-EPS
C     WRITE(6,*)FACT
      IF(FACT.LT.Ø.)FACT=1.E-5Ø
      DERY(1)=-1.*Y(1)*(1.+Y(1))*G1P/G1+Y(1)/(1.-Y(2))*(C*(1.-Y(1))/MØ
     1-B*Y(2)*(1.+Y(1))+2.*Y(1)*G1*FACT**(-.5*(GAM+1.))/MØ)
C
C
   6Ø CONTINUE
      RETURN
      END
      SUBROUTINE GILL(N)
C     SUBROUTINE GILL(N,Q,DERIV)
C     DOUBLE Y(N),DERY(N),Q(N),G1,G1P,XK,DY
      DOUBLE Y(2Ø),DERY(2Ø),Q(2Ø),G1,G1P,XK,DY
      COMMON /G/ Q,A(4),B(4),C(4)
      DATA A(1),B(1),C(1),C(4)/Ø.5,-1.Ø,-Ø.5,-Ø.5/
      DO 1Ø I=1,N
   1Ø Q(I)=Ø.Ø
      C1=1.Ø/SQRT(2.Ø)
      A(2)=1.Ø-C1
      A(3)=1.Ø+C1
      A(4)=1.Ø/6.Ø
      B(2)=-A(2)
      B(3)=-A(3)
      B(4)=-1.Ø/3.Ø
      C(2)=B(2)
      C(3)=B(3)
      RETURN
      END
      SUBROUTINE GILL1(DX,X,Y,DERY)
C     CALL GILL1(DX,X,Y,DERY)
      DOUBLE Y(2Ø),DERY(2Ø),Q(2Ø),G1,G1P,XK,DY
      COMMON /G/ Q,A(4),B(4),C(4)
      DO 3Ø I=1,4
      IF(I.EQ.2.OR.I.EQ.4) X=X+Ø.5*DX
C     CALL DERIV (X,Y,DERY,G1,G1P)
      NSUB=2
      CALL DERIV(X,Y,DERY,G1,G1P,NSUB)
      DO 3Ø J=1,N
      XK=DX*DERY(J)
      DY=A(I)*XK+B(I)*Q(J)
      Y(J)=Y(J)+DY
      Q(J)=Q(J)+3.Ø*DY+C(I)*XK
   3Ø CONTINUE
```

```
      RETURN
      END
      SUBROUTINE RATEAU(TSTAR,T2Ø,EJECTO,II,J)
      REAL MØ,LAMM,L,MP,MACHNO
      COMMON/WORKA/LAMM,GAM,EPS,MØ,BØ,CØ,DØ,KPMAX
      COMMON/WORKB/THETA(5ØØ),Z(5ØØ),H1(5ØØ),H1P(5ØØ),THETAP(5ØØ),
     1 TTAU(5ØØ),FEJECT(5ØØ)
      COMMON/WORKC/TEFF,ETA,A,L,MP,VØ,ALMP,R
      COMMON/WORKD/PE(5Ø),UE(5Ø),TE(5Ø),RHOE(5Ø),TIME(5Ø),
     1 TEMP(5Ø), FKP(5Ø),CO2(5Ø),CO(5Ø),H2O(5Ø),H2(5Ø)
      DATA DELTAT/1.E-Ø3/
      DATA IWRITE/6/
      TSTAR = TSTAR/1ØØØ.
      THET = (.5*(GAM+1.))**((GAM+1.)/(GAM-1.))/GAM
      THET = THET/R/TEFF/(1.+LAMM/6.)/(1.-ETA*LAMM)**(GAM-1.)
      THET = 2.*L*(1.+.Ø13*ETA/ALMP)/(GAM-1.)*SQRT(THET)
      TØ = ((1.+LAMM/6.)*TEFF/T2Ø)**(1./(GAM-1.))
      TØ = TØ*(ALMP-ETA)/(ALMP+1.Ø7*ETA)
      TØ = TØ + 2.Ø7*ETA/(ALMP+1.Ø7*ETA)
      TØ = THET*(TØ**(.5*(GAM-1.)) - 1.)
      T = TSTAR - DELTAT
      EJECT = FEJECT(II)
      J = Ø
   1Ø J = J + 1
      T = T + DELTAT
      TMSEC = 1ØØØ.*T
      TREPLC = T - TSTAR + TØ
      RHO2 = (1. + TREPLC/THET)**(2./(GAM-1.))
      RHO2 = (ALMP + 1.Ø7*ETA)*RHO2 - 1.Ø7*ETA
      RHO2 = 1./RHO2
      P2 = R*TEFF*(1.+LAMM/6.)
      P2 = P2*(ALMP-ETA)**(GAM-1.)
      P2 = P2/(1./RHO2-ETA)**GAM
      T2 = P2*(1./RHO2-ETA)/R
      V2 = (ALMP-ETA)/(1./RHO2-ETA)
      V2 = VØ/MØ/(1.-ETA*RHO2)*V2**(.5*(GAM-1.))
      SONICV = SQRT(GAM*R*T2)
      MACHNO = V2/SONICV
      P2ATM = P2/1Ø133Ø.
      PE(J) = P2ATM
      UE(J) = V2
      TE(J) = T2
      RHOE(J) = RHO2
      TIME(J) = TMSEC
C
C  DETERMINE THE REACTION RATE CONSTANT FKP
C
      TA = T2/P2ATM**((GAM-1.)/GAM)
      DO 2Ø I=1,KPMAX
      IF(TA.GE.TEMP(I)) GO TO 2Ø
      IF(I.LE.1) GO TO 3Ø
      SLOPE = (FKP(I) - FKP(I-1))/(TEMP(I) - TEMP(I-1))
      FKPP = SLOPE*(TA - TEMP(I)) + FKP(I)
      GO TO 4Ø
   2Ø CONTINUE
```

```
   3Ø WRITE(IWRITE,1ØØØ) TMSEC,TA
 1ØØØ FORMAT(' EXIT PLANE TEMPERATURE T2 IS OUTSIDE THE RATE',
     1 ' CONSTANT INTERPOLATION TABLE RANGE'/' COMPUTATION',
     2 ' TERMINATED WITH TIME =',F1Ø.3,' ,T2 =',F1Ø.3/)
   4Ø CONTINUE
C
      AA = (DØ*FKPP +  BØ + CØ)**2 + 4.*BØ*CØ*(FKPP-1.)
      AA = SQRT(AA) - DØ*FKPP - BØ - CØ
      AA = AA/(2.*(FKPP-1.))
      CO2(J) = AA
      CO(J) = BØ - AA
      H2O(J) = CØ - AA
      H2(J) = DØ + AA
C
      IF(J.EQ.1) GO TO 5Ø
      EJECTN = .5*A/MP*RHO2*V2*DELTAT
      EJECT = EJECT + EJECTN + EJECTO
      EJECTO = EJECTN
   5Ø WRITE(IWRITE,1Ø1Ø) TMSEC,RHO2,V2,P2,P2ATM,T2,SONICV,MACHNO,EJECT
 1Ø1Ø FORMAT(' ',1P9G13.4)
      IF(P2ATM.LE.1.) RETURN
      GO TO 1Ø
      END
C
      SUBROUTINE MACHN(R,FM,PHI,GAM,XI)
C
C MACHN CALCULATES THE MACH NUMBER GIVEN THE AXIAL DIATANCE
C FROM THE MUZZLE BY HALF INTERVAL SEARCH
C
      DATA IWRITE/6/
      DATA EPS/.Ø1/
      F(X) = SQRT(.49*GAM*(2.+(GAM-1.)*X*X)**(GAM/(GAM-1.))/
     1 (1. + .197*PHI**.65)**2/(2.*GAM*X*X - GAM + 1.)/
     2 (GAM+1.)**(1./(GAM-1.)))
      FMIN = 1.
      FMAX = 1.
      DO 1Ø I=1,2Ø
      FMAX = FMAX + FMAX*FMAX
      IF(F(FMAX).GE.XI) GO TO 3Ø
   1Ø CONTINUE
      DO 2Ø I=1,2ØØ
      FM = .5*(FMIN + FMAX)
      DELTA = F(FM) - R
      IF(ABS(DELTA).LE.EPS) RETURN
      IF(DELTA.LE.Ø.) FMIN = FM
      IF(DELTA.GT.Ø.) FMAX = FM
   2Ø CONTINUE
   3Ø CONTINUE
      WRITE(IWRITE,1ØØØ) FMIN,FMAX,FM,R,DELTA
 1ØØØ FORMAT('ØWARNING-SUBROUTINE MACHN''S CALCULATION',
     1 ' OF MACH NUMBER HAS NOT CONVERGED AFTER 2ØØ ITERATIONS'/
     2' FMIN =',1PG1Ø.3,' FMAX =',G1Ø.3,' FM =',G1Ø.3,' R =',
     3 G1Ø.3,' DELTA =',G1Ø.3)
      STOP
      END
```

APPENDIX F

MTOB PROGRAM LISTING

```
      PROGRAM MTOB(INPUT,OUTPUT,TAPE9,TAPE4,TAPE8,TAPE6=OUTPUT)
C
C TAPE8 IS OUTPUT TAPE FOR BLAKE, CONCEN, AND LAPP
C TAPE9 IS INPUT TAPE FROM MEFF
C TAPE4 IS INPUT BOILERPLATE FOR THE APPROPRIATE GAS
C
      DIMENSION A(3Ø,8Ø),TITLE(2Ø)
      REWIND 4
      REWIND 8
      REWIND 9
C
C READ THE RESULTS OF THE MEFF CALCULATION
      READ(9,4ØØ)TITLE
      READ(9,3ØØ)T1,T2,T3,P,V,ALPHA,RADIUS,XMAX,PRNT,FDL,KEY
C
C NOW READ THE BLAKE BOILERPLATE
      DO 2Ø I=1,3Ø
      IF(EOF(4))3Ø,2Ø
   2Ø READ(4,1ØØ)(A(I,J),J=1,8Ø)
C
C HERE ONCE BOILERPLATE FILE IS READ
   3Ø II=I-2
C
      DO 4Ø K=1,II
   4Ø WRITE(8,1ØØ)(A(K,J),J=1,8Ø)
C
C NOW FOR THE SPECIAL LINES
C
   5Ø WRITE(8,12Ø)
  12Ø FORMAT(9HPRL,CON,2)
      WRITE(8,11Ø)T1
  11Ø FORMAT(11HPOI,P,1.,T,,F8.3)
      WRITE(8,13Ø)P,T2
  13Ø FORMAT(6HPOI,P,,F8.3,3H,T,,F8.3)
      WRITE(8,17Ø)
  17Ø FORMAT(4HQUIT)
      WRITE(8,18Ø)ALPHA
  18Ø FORMAT(F8.3)
      WRITE(8,4ØØ) TITLE
      WRITE(8,19Ø)RADIUS,XMAX,PRNT
  19Ø FORMAT(3E1Ø.3)
      WRITE(8,21Ø)FDL,KEY
  21Ø FORMAT(F8.3,I1)
      WRITE(8,2ØØ)T3,V
  2ØØ FORMAT(2F8.3,/,4H*EOI)
  3ØØ FORMAT(1ØF8.3,I1)
  1ØØ FORMAT(8ØA1)
  4ØØ FORMAT(2ØA4)
      END
```

APPENDIX G

BOIL LISTING

```
TIT,M3ØA1
PRL,CON,2
REJ,N,K2SO4,C,C2,CH,CH2O,HNO3
REJ,C(S),K2SO4$
REJ,KOH$,KO2$,K2O2$
REJ,H2S,S2O,SO2,K$,K2O,K2O2
REJ,KCO$,KSO$,K2O$,K$
REJ,K2CO3$
REJ,K2S$
UNI,ENG
CM2,NC126Ø,27.9,NG,22.42,NQ,46.84,EC,1.49,KS,1.,
ALC,.25,C,.1
```

APPENDIX H

CONCEN PROGRAM LISTING

```
      PROGRAM CONCEN(INPUT,OUTPUT,TAPE1,TAPE2,TAPE5=INPUT,
     + TAPE6=OUTPUT,TAPE8)
C
C 13 SPECIES
C
      DIMENSION NAM(17),CONC(17,2),NA(2,29),CO(2,29)
      DIMENSION CON(17),SUM(2)
      DATA CONST/'CONST'/
C
C THE NAME OF EACH SPECIES MUST BE 4 CHARACTERS
C
      DATA NAM/' H2O','  CO','  H2','  N2',' CO2','   H','  OH','   O',
     +'  O2','   K',' KOH',' KO2',' HO2'/
      REWIND 1
      REWIND 2
      READ(8,300)ALPHA
      NSPEC=13
      K=0
      I=0
      SUM(1)=0.
      SUM(2)=0.
    1 READ(1,200)ALINE
      IF(ALINE.NE.CONST)GOTO 1
      I=I+1
      READ(1,200)JUNK
      DO 10 J=1,29
      READ(1,100)NA(I,J),CO(I,J)
      IF(NA(I,J).EQ.'    ')GOTO 20
   10 CONTINUE
   20 IF(I.EQ.1)GOTO 1
   50 K=K+1
      DO 30 I=1,NSPEC
      DO 40 J=1,29
      IF(NA(K,J).EQ.NAM(I))CONC(I,K)=CO(K,J)
   40 CONTINUE
   30 CONTINUE
      DO 60 L=1,NSPEC
   60 CONTINUE
      IF(K.EQ.1)GOTO 50
      DO 70 I=1,2
      DO 80 J=1,NSPEC
      SUM(I)=SUM(I)+CO(I,J)
   80 CONTINUE
   70 CONTINUE
      WRITE(6,400)
      WRITE(6,500)ALPHA
      DO 90 I=1,NSPEC
      CON(I)=(1.-ALPHA)*(CONC(I,1)/SUM(1))+ALPHA*(CONC(I,2)/SUM(2))
      WRITE(6,400)NAM(I),CON(I)
   90 CONTINUE
      WRITE(2,700)(CON(I),I=1,NSPEC)
      WRITE(6,600)
      STOP
  100 FORMAT(4X,A4,14X,1PE11.5)
  200 FORMAT(9X,A5)
```

```
300 FORMAT(F8.3)
400 FORMAT(2X,A4,5X,1PE10.3)
500 FORMAT(1H1,2X,' ALPHA= ',F5.3)
600 FORMAT(1H1)
700 FORMAT(7E10.4)
    END
```

APPENDIX I

LASTDA DATA LISTING

```
   13    13     6    42     0      0      0   200     0    22

        0.      99.99       9.99          1.          1.   999.999          1.
   .1E-10        .999
     1.00       999.9       294.       9999.       0.1                  200.
   .1E-50      .1E-50     .1E-50         .79     .00032    .1E-50     .1E-50
   .1E-50         .21     .1E-50      .1E-50     .1E-50    .1E-50
H2O        18.016    -57.7979
     100.       7.961     52.202      -1.581       200.      7.969     45.837      -0.784
     400.       8.186     45.422       0.825       600.      8.676     46.710       2.509
     800.       9.246     48.089       4.300      1000.      9.851     49.382       6.209
    1200.      10.444     50.575       8.240      1400.     10.987     51.675      10.384
    1600.      11.462     52.698      12.630      1800.     11.869     53.652      14.964
    2000.      12.214     54.548      17.373      2200.     12.505     55.392      19.846
    2400.      12.753     56.190      22.372      2600.     12.965     56.947      24.945
    2800.      13.146     57.667      27.556      3000.     13.304     58.354      30.201
    3200.      13.441     59.010      32.876      3400.     13.562     59.639      35.577
    3600.      13.669     60.242      38.300      3800.     13.764     60.821      41.043
    4000.      13.850     61.379      43.805      4200.     13.927     61.917      46.583
CO       28.01055      -26.42
     100.       6.956     53.401      -1.379       200.      6.957     47.851      -0.683
     400.       7.013     47.488       0.711       600.      7.276     48.591       2.137
     800.       7.624     49.759       3.627      1000.      7.931     50.845       5.183
    1200.       8.168     51.834       6.794      1400.      8.346     52.736       8.446
    1600.       8.480     53.562      10.130      1800.      8.583     54.322      11.836
    2000.       8.664     55.026      13.561      2200.      8.728     55.680      15.301
    2400.       8.781     56.292      17.052      2600.      8.825     56.866      18.813
    2800.       8.863     57.407      20.582      3000.      8.895     57.917      22.357
    3200.       8.924     58.401      24.139      3400.      8.949     58.861      25.927
    3600.       8.973     59.299      27.719      3800.      8.994     59.717      29.516
    4000.       9.014     60.117      31.316      4200.      9.033     60.501      33.121
H2           2.016        0.0
     100.       5.393     37.035      -1.265       200.      6.518     31.831      -0.662
     400.       6.975     31.480       0.707       600.      7.009     32.573       2.106
     800.       7.087     33.715       3.514      1000.      7.219     34.758       4.944
    1200.       7.390     35.696       6.404      1400.      7.600     36.543       7.902
    1600.       7.823     37.314       9.446      1800.      8.016     38.022      11.030
    2000.       8.195     38.678      12.651      2200.      8.358     39.290      14.307
    2400.       8.506     39.863      15.993      2600.      8.639     40.402      17.708
    2800.       8.757     40.912      19.448      3000.      8.859     41.395      21.210
    3200.       8.962     41.855      22.992      3400.      9.061     42.294      24.794
    3600.       9.158     42.714      26.616      3800.      9.252     43.116      28.457
    4000.       9.342     43.502      30.317      4200.      9.429     43.874      32.194
N2        28.0134         0.0
     100.       6.956     51.957      -1.379       200.      6.957     46.407      -0.683
     400.       6.990     46.043       0.710       600.      7.196     47.143       2.125
     800.       7.512     48.303       3.596      1000.      7.815     49.378       5.129
    1200.       8.061     50.357       6.718      1400.      8.252     51.248       8.350
    1600.       8.398     52.065      10.015      1800.      8.512     52.816      11.707
    2000.       8.601     53.513      13.418      2200.      8.672     54.160      15.146
    2400.       8.731     54.766      16.886      2600.      8.779     55.335      18.638
    2800.       8.820     55.870      20.398      3000.      8.855     56.376      22.165
    3200.       8.886     56.856      23.939      3400.      8.914     57.312      25.719
    3600.       8.939     57.747      27.505      3800.      8.962     58.162      29.295
    4000.       8.983     58.559      31.089      4200.      9.002     58.940      32.888
```

CO2	44.053	-94.054						
	100.	6.981	58.188	-1.543	200.	7.734	51.849	-0.816
	400.	9.877	51.434	0.958	600.	11.310	52.981	3.087
	800.	12.293	54.706	5.453	1000.	12.980	56.359	7.984
	1200.	13.466	57.896	10.632	1400.	13.815	59.315	13.362
	1600.	14.074	60.627	16.152	1800.	14.269	61.843	18.987
	2000.	14.424	62.974	21.857	2200.	14.547	64.031	24.755
	2400.	14.643	65.023	27.674	2600.	14.734	65.956	30.613
	2800.	14.807	66.836	33.567	3000.	14.873	67.670	36.535
	3200.	14.930	68.461	39.515	3400.	14.982	69.215	42.507
	3600.	15.030	69.933	45.508	3800.	15.075	70.620	48.518
	4000.	15.119	71.278	51.538	4200.	15.159	71.909	54.566
H	1.00797E0	52.1						
	100.	4.968	31.809	-0.984	200.	4.968	27.847	-0.488
	400.	4.968	27.587	0.506	600.	4.968	28.367	1.500
	800.	4.968	29.179	2.493	1000.	4.968	29.917	3.487
	1200.	4.968	30.576	4.481	1400.	4.968	31.166	5.474
	1600.	4.968	31.697	6.468	1800.	4.968	32.179	7.461
	2000.	4.968	32.621	8.455	2200.	4.968	33.027	9.449
	2400.	4.968	33.403	10.442	2600.	4.968	33.753	11.436
	2800.	4.968	34.081	12.430	3000.	4.968	34.388	13.423
	3200.	4.968	34.678	14.417	3400.	4.968	34.952	15.410
	3600.	4.968	35.212	16.404	3800.	4.968	35.459	17.398
	4000.	4.968	35.694	18.391	4200.	4.968	35.919	19.385
OH	17.0074	9.492						
	100.	7.798	50.398	-1.467	200.	7.356	44.541	-0.711
	400.	7.087	44.160	0.725	600.	7.057	45.275	2.137
	800.	7.150	46.432	3.556	1000.	7.332	47.488	5.003
	1200.	7.549	48.437	6.491	1400.	7.766	49.296	8.023
	1600.	7.963	50.079	9.596	1800.	8.137	50.799	11.207
	2000.	8.286	51.466	12.849	2200.	8.415	52.087	14.520
	2400.	8.526	52.668	16.214	2600.	8.622	53.214	17.929
	2800.	8.706	53.730	19.622	3000.	8.780	54.218	21.411
	3200.	8.846	54.682	23.174	3400.	8.905	55.124	24.949
	3600.	8.959	55.546	26.735	3800.	9.009	55.950	28.532
	4000.	9.054	56.337	30.339	4200.	9.097	56.709	32.154
O	16.000	59.559						
	100.	5.666	43.266	-1.080	200.	5.434	38.953	-0.523
	400.	5.135	38.672	0.528	600.	5.049	39.480	1.544
	800.	5.015	40.313	2.550	1000.	4.999	41.067	3.552
	1200.	4.990	41.737	4.551	1400.	4.984	42.335	5.548
	1600.	4.981	42.873	6.544	1800.	4.979	43.361	7.540
	2000.	4.978	43.806	8.536	2200.	4.979	44.216	9.532
	2400.	4.981	44.596	10.527	2600.	4.986	44.948	11.524
	2800.	4.994	45.278	12.522	3000.	5.004	45.588	13.522
	3200.	5.017	45.880	14.524	3400.	5.033	46.156	15.529
	3600.	5.050	46.418	16.537	3800.	5.070	46.667	17.549
	4000.	5.091	46.904	18.565	4200.	5.114	47.131	19.586
O2	31.9988	0.0						
	100.	6.958	55.205	-1.381	200.	6.961	49.643	-0.685
	400.	7.196	49.282	0.724	600.	7.670	50.414	2.210
	800.	8.063	51.629	3.786	1000.	8.336	52.765	5.427
	1200.	8.527	53.801	7.114	1400.	8.674	54.744	8.835
	1600.	8.800	55.608	10.583	1800.	8.916	56.401	12.354
	2000.	9.029	57.136	14.149	2200.	9.139	57.819	15.966

	2400.	9.248	58.457	17.804	2600.	9.354	59.057	19.664
	2800.	9.455	59.622	21.545	3000.	9.551	60.157	23.446
	3200.	9.640	60.665	25.365	3400.	9.723	61.149	27.302
	3600.	9.799	61.611	29.254	3800.	9.869	62.053	31.221
	4000.	9.932	62.476	33.201	4200.	9.988	62.883	35.193
K	39.100	21.31						
	100.	4.968	42.714	-.984	200.	4.968	38.751	-.488
	400.	4.968	38.492	.506	600.	4.968	39.272	1.500
	800.	4.968	40.084	2.493	1000.	4.968	40.822	3.487
	1200.	4.968	41.481	4.481	1400.	4.970	42.070	5.474
	1600.	4.975	42.602	6.469	1800.	4.988	43.084	7.465
	2000.	5.013	43.526	8.465	2200.	5.057	43.932	9.471
	2400.	5.122	44.310	10.489	2600.	5.213	44.662	11.522
	2800.	5.334	44.993	12.576	3000.	5.489	45.305	13.658
	3200.	5.685	45.601	14.775	3400.	5.932	45.883	15.935
	3600.	6.242	46.153	17.152	3800.	6.630	46.412	18.438
	4000.	7.111	46.664	19.810	4200.	7.701	46.908	21.289
KOH	56.109	-55.6						
	100.	7.874	65.898	-2.017	200.	10.439	57.500	-1.090
	400.	12.136	56.932	1.212	600.	12.578	58.830	3.690
	800.	12.835	60.845	6.232	1000.	13.083	62.702	8.824
	1200.	13.327	64.379	11.465	1400.	13.551	65.895	14.154
	1600.	13.746	67.275	16.884	1800.	13.911	68.539	19.650
	2000.	14.048	69.706	22.446	2200.	14.162	70.788	25.268
	2400.	14.257	71.798	28.110	2600.	14.336	72.743	30.970
	2800.	14.403	73.632	33.844	3000.	14.459	74.472	36.730
	3200.	14.506	75.266	39.626	3400.	14.547	76.021	42.532
	3600.	14.582	76.739	45.445	3800.	14.612	77.425	48.364
	4000.	14.638	78.080	51.289	4200.	14.661	78.708	54.219
KO2	71.1	-15.0						
	100.	9.925	75.72	-2.133	200.	10.810	67.02	-1.095
	400.	12.086	66.45	1.205	600.	12.830	68.35	3.704
	800.	13.216	70.38	6.313	1000.	13.438	72.26	8.979
	1200.	13.587	73.97	11.682	1400.	13.687	75.52	14.411
	1600.	13.749	76.92	17.155	1800.	13.784	78.20	19.908
	2000.	13.799	79.38	22.667	2200.	13.803	80.47	25.427
	2400.	13.801	81.49	28.188	2600.	13.797	82.43	30.948
	2800.	13.797	83.32	33.707	3000.	13.802	84.16	36.467
	3200.	13.814	84.94	39.228	3400.	13.831	85.69	41.993
	3600.	13.855	86.40	44.761	3800.	13.881	87.07	47.535
	4000.	13.905	87.72	50.313	4200.	13.925	88.33	53.097
HO2	33.008	0.5						
	100.	7.949	61.574	-1.596	200.	8.003	55.132	-0.799
	400.	8.907	54.717	0.877	600.	9.980	56.116	2.771
	800.	10.769	57.657	4.850	1000.	11.365	59.123	7.066
	1200.	11.831	60.481	9.387	1400.	12.197	61.734	11.791
	1600.	12.485	62.891	14.261	1800.	12.714	63.965	16.782
	2000.	12.895	64.966	19.343	2200.	13.041	65.902	21.937
	2400.	13.160	66.781	24.558	2600.	13.256	67.610	27.200
	2800.	13.336	68.393	29.859	3000.	13.403	69.135	32.534
	3200.	13.459	69.840	35.220	3400.	13.507	70.511	37.917
	3600.	13.547	71.153	40.622	3800.	13.582	71.766	43.335
	4000.	13.612	72.354	46.055	4200.	13.638	72.918	48.780

CO	+0	+M	=CO2	+M	26	7.0E-33	0.	-4369.
CO	+02	+	=CO2	+0	15	4.2E-12	0.	-47664.

O	+O	+M	=O2	+M	25	3.ØE-34	Ø.	1792.Ø
CO	+OH	+	=CO2	+H	16	2.8E-17	-1.3	66Ø.Ø
OH	+H2	+	=H2O	+H	16	1.9ØE-15	-1.3	-3626.
H	+O2	+	=OH	+O	15	2.4ØE-1Ø	Ø.	-16393.
O	+H2	+	=OH	+H	16	3.ØE-14	-1.	-89Ø2.
OH	+OH	+	=H2O	+O	15	1.Ø5E-11	Ø.	-1Ø93.
H	+H	+M	=H2	+M	22	3.ØØE-3Ø	1.	Ø.
H	+OH	+M	=H2O	+M	23	1.ØØE-25	2.	Ø.
H	+O2	+M	=HO2	+M	25	1.5E-32	Ø.	994.
H	+HO2	+	=OH	+OH	15	1.7E-1Ø	Ø.	-994.
CO	+HO2	+	=CO2	+OH	15	2.5E-1Ø	Ø.	-23645.
H	+HO2	+	=H2	+O2	15	4.2E-11	Ø.	-695.
H	+HO2	+	=H2O	+O	15	8.5E-12	Ø.	-994.
OH	+HO2	+	=H2O	+O2	11	3.ØE-11	Ø.	Ø.
O	+HO2	+	=OH	+O2	11	3.5E-11	Ø.	Ø.
O	+H	+M	=OH	+M	22	1.ØE-29	1.	Ø.
HO2	+H2	+	=H2O	+OH	15	1.ØE-12	Ø.	-18678.
H	+KOH	+	=H2O	+K	15	1.8E-11	Ø.	-1987.
K	+OH	+M	=KOH	+M	22	1.5E-27	1.	Ø.
KO2	+OH	+	=KOH	+O2	11	2.ØE-11	Ø.	Ø.
K	+O2	+M	=KO2	+M	22	3.ØE-3Ø	1.	Ø.
K	+HO2	+	=KO2	+H	15	1.ØE-11	Ø.	-13ØØØ.
KO2	+H2	+	=KOH	+OH	15	3.ØE-12	Ø.	-1987Ø.

APPENDIX J

LAPP PROGRAM LISTING

```
C
C RELEASE VERSION OF LAPP MODIFIED TO ACCEPT UP THROUGH 49 REACTIONS.
C     MARCH 1983
C
C
      PROGRAM LAPP(INPUT,OUTPUT,TAPE2,TAPE3,TAPE5=INPUT,TAPE6=OUTPUT,
     + TAPE7,TAPE8,TAPE1Ø,TAPE11,TAPE12)
C
C TAPE2 IS INPUT FROM PROGRAM CONCEN
C TAPE3 IS INPUT FROM FILE OF LAPP DATA
C TAPE8 IS INPUT FROM PROGRAM MTOB
C
C**********************************************************************
C**********                                                          **
C**********      AXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY    **
C**********               AEROCHEM RESEARCH LABORATORIES             **
C**********                    PRINCETON, N. J.                      **
C**********                                                          **
C**********************************************************************
      DIMENSION A(3Ø),RHO(3Ø),Y(3Ø),T(3Ø),PSI(3Ø),RT(3Ø),SUM(3Ø),AR(25),
     1HSTAT(3Ø),H(25,3Ø),ALPHA(25,3Ø),RALPHA(25,3Ø),CP(25,3Ø),SIGMA(3Ø),
     2           WTMOLE(25),CPBAR(3Ø),C(25,9),AID(25),ETA(3Ø),RATIO(3Ø),
     3RU(3Ø),U(3Ø),TITLE(12),XLE(3Ø),XMU(3Ø)           ,G(25),WTMIX(3Ø),
     4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,3Ø),SAVET(3Ø),SAVEU(3Ø),
     5          IRR(49),FREQ(3Ø),SAVEA(25,3Ø),             PC(4),ZID(5),
     6          ECC(3Ø),HOUT(3Ø),YOUT(3Ø),RHOOUT(3Ø),XMUOUT(3Ø),XLT(3Ø),
     7T4(3Ø),TFDG(3Ø),IRT(49),RP(49,3Ø),RM(49,3Ø)
      DIMENSION XAME(6), ISAVE(6), FREQA(6), ALOC(5Ø,6)
      DIMENSION TTB(3Ø,24)    ,CPTB(25,3Ø),HTB(25,3Ø),GTB(25,3Ø),HF(25)
      DIMENSION TABLE(16),ZSPEC(16)
      COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
      COMMON/UNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,
     *NUNITG,NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NUNITN,
     *NOUT,NDBG,NNNOUT
      COMMON/A/ CM(25,25,26),CM1(25,25),QX(25,26),QX1(25)
      COMMON/C/ IZSPEC,ISPEC(16)
      COMMON  A      , RHO    , Y      , T      , PSI    , RT
      COMMON  SUM    , AR     , HSTAT  , H      , ALPHA  , RALPHA
      COMMON  CP     , SIGMA           , WTMOLE , CPBAR  , C
      COMMON  AID    , ETA    , RATIO  , RU     , U      , TITLE
      COMMON  XLE    , XMU    ,          G      , WTMIX  , WDOT
      COMMON  SAVEU  , SAVET  , WM     , WP     , RC
      COMMON           SAVEA  ,          PC     , X      , XMAX
      COMMON  PRNT   , DXMIN  , DX     , FDL    , DELPSI , RJ
      COMMON  XK2    , P      , ZID    , FREQ   , ECC    , DPDX
      COMMON  YOUT   , HOUT   , RHOOUT , IRRR   , IRR    , IFINIS
      COMMON  IPAGE  , MPSI   , MY     , NS     , NR     , IEDGE
      COMMON  ITURB  , IPRESS , NPSI   , ITEST  , ITER   , IECC
      COMMON  IRT    , XMUOUT , XLT    , T4     , TFDG   , IOUT
      COMMON  IOUT1  , IOUT2  ,RP      , RM     , ISAVE  , IPUNCH
      COMMON TKINET,NFREQA,ALOC,FREQA,QQ1ØØ,QQ2ØØ,QQ3ØØ,QQ4ØØ
C
C**** SETTING XAME FOR THOSE SPECIES INVOLVED IN COLLISION FREQ. CALC.
C
      DATA XAME(1)/6HCO    /
```

```
      DATA XAME(2)/6HCO2   /
      DATA XAME(3)/6HH2O   /
      DATA XAME(4)/6HH2    /
      DATA XAME(5)/6HN2    /
      DATA XAME(6)/6HHCL   /
      DATA TABLE/8HCO      ,8HHCL     ,8HH2O     ,8HOH      ,
     1           8HCO2     ,8HHF      ,8HCN      ,8HO       ,
     2           8HBF      ,8HBFO     ,8HBHO2    ,8HBF2     ,
     3           8HBF3     ,8HBO      ,8H        ,8HAL2O3   /
C
CCCCC COMMENT OUT NAMELIST DEFINITION WHICH FOLLOWS IF PROCESS NAMELIST
CCCCC BY CALLS TO SUBROUTINE NMLST....ALSO COMMENT OUT NORMAL READS
CCCCC AND WRITES FOR IBM SUPPORTED NAMELIST
CCCCC NAMELIST/NUNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,NUNITG,
CCCCC*NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NOUT,NDBG
C
C     INITIALIZE VARIABLES
      AMULT=Ø.3Ø48
      AMULT3=14.5939
      JPROC=2
      NUNITA=2
      NUNITB=3
      NUNITC=5
      NUNITD=7
      NUNITE=7
      NUNITF=8
      NUNITG=Ø
      NUNITH=Ø
      NUNITI=Ø
      NUNITJ=Ø
      NUNITK=Ø
      NUNITL=Ø
      NUNITM=Ø
      NUNITN=5
      NOUT=6
      NNOUT=6
      NNNOUT=1Ø
      NDBG=6
C
      AV=6.Ø25E23
C... SET CONVERSION TO ENGLISH UNITS MULTIPLIERS
      AMULT1=AMULT*AMULT
      AMULT2=AMULT*AMULT1
      AMULT3=SQRT(AMULT3)
    4 IFINIS=Ø
      DO 9999 I=1,8536
 9999 A(I)=Ø.Ø
      DO 3ØØ I = 1,6
  3ØØ ISAVE(I) = Ø
      R=82.Ø6
C..... BEGIN TO INPUT FILE DESIGNATED BY NUNITB
      READ  (NUNITF,333)(TITLE(I),I=1,1Ø)
      IF(NUNITM.LT.Ø)WRITE(NNOUT,333) (TITLE(I),I=1,1Ø)
C
C     NS= NO. OF SPECIES
```

```
C     NR= NO. OF REACTIONS
C
C
      READ(NUNITB,100) MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,
     *IPRESS,NT
      IF(NUNITM.LT.0)WRITE(NNOUT,100) MPSI,NS,ITURB,NR,IOUT1,IOUT2,
     *IPUNCH,ITIME,IPRESS,NT
      READ (NUNITB,111)  (FREQA(I), I=1,6)
      IF(NUNITM.LT.0) WRITE(NNOUT,111) (FREQA(I),I=1,6)
      DO 113 I=1,6
      IF (FREQA(I)) 113, 114, 113
  113 CONTINUE
      I=7
  114 NFREQA = I-1
      NPSI=MPSI-1
      READ  (NUNITB,1000)X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2
      READ(NUNITF,1000)RJ,XMAX,PRNT
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK
      X=X/AMULT
      XMAX=XMAX/AMULT
      PRNT=PRNT/AMULT
      RJ=RJ/AMULT
      DX=0.1*RJ
C
C     INPUT MINIMUM STEPSIZE LIMIT (DXMIN)
C
      READ(NUNITB,555) DXMIN,FDL,PC(1),PC(2),PC(3),PC(4),THOT,TCOOL
      READ(NUNITF,556)FDL,KEY
  556 FORMAT(F8.3,I1)
      IF(NUNITM.LT.0) WRITE(NNOUT,555)DXMIN,FDL,(PC(KI),KI=1,4),THOT,
     *TCOOL
      IF(KEY.EQ.1)GOTO 98765
      NOUT=10
      NNOUT=10
      NCBG=10
      NNNOUT=6
98765 DXMIN=DXMIN/AMULT
      PC(2)=PC(2)*AMULT
      PC(3)=PC(3)*AMULT1
      PC(4)=PC(4)*AMULT2
      READ  (NUNITB,1000)P,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET
      READ(NUNITF,987)T(1),U(1)
  987 FORMAT(2F8.3)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)P,T(1),T(MPSI),U(1),U(MPSI),
     *DELPSI,TKINET
      U(1)=U(1)/AMULT
      U(MPSI)=U(MPSI)/AMULT
      DELPSI=DELPSI/AMULT3
      IF(TKINET.EQ.0.0) TKINET = 400.0
C
C**** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILE TIME
C
      ILIMIT = 60*ITIME
      IDIFFT = 0
      CALL TICK(ISECST)
```

```
      IF((ISECST+6Ø*ITIME).GT.864ØØ) IDIFFT = 864ØØ-ISECST
      UNIT = U(1)
      IQ77 = 2
      USUBØ1 = Ø.Ø
C
C     TURBULENCE MODELS
C
      IF (ITURB - 3) 86ØØ,9Ø1Ø,9Ø1Ø
 86ØØ IF (ITURB - 1) 9Ø11,9Ø1Ø,9Ø11
 9Ø1Ø USUBØ1 = Ø.95*   (U(1)-U(MPSI)) + U(MPSI)
 9Ø11 CONTINUE
      IF(DELPSI) 3Ø11,3Ø12,3Ø11
C
C**** READING OF CENTERLINE CONCENTRATIONS FROM FILE PRODUCED
C**** BY BLAKE AND CONCEN.
C
 3Ø12 READ  (NUNITA,1ØØØ)(ALPHA(J,1),J=1,NS)
C
C BE SURE NO DENSITIES ARE ZERO
      DO 7777 IJK=1,NS
      ALPHA(IJK,1)=AMAX1(ALPHA(IJK,1),1.E-99)
 7777 CONTINUE
C
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1ØØØ)(ALPHA(J,1),J=1,NS)
C
C**** NOW READ THE CONCENTRATIONS ON THE EDGES - AMBIENT AIR.
C
      READ(NUNITB,1ØØØ)(ALPHA(J,MPSI),J=1,NS)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1ØØØ)(ALPHA(J,MPSI),J=1,NS)
      MMOD=MPSI-2
      DO 4ØØ1 I=1,MMOD
      T(I)=T(1)
      U(I)=U(1)
      DO 4ØØ1 J=1,NS
 4ØØ1 ALPHA(J,I)=ALPHA(J,1)
      DO 4ØØ2 J=1,NS
 4ØØ2 ALPHA(J,NPSI)=ALPHA(J,MPSI)
      GO TO 3Ø15
 3Ø11 READ  (NUNITB,1ØØØ)(T(I),I=1,MPSI)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1ØØØ)(T(I),I=1,MPSI)
      READ  (NUNITB,1ØØØ)(U(I),I=1,MPSI)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1ØØØ)(U(I),I=1,MPSI)
      DO 7 I=1,MPSI
      U(I)=U(I)/AMULT
      READ  (NUNITB,1ØØØ)(ALPHA(J,I),J=1,NS)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1ØØØ)(ALPHA(J,I),J=1,NS)
    7 CONTINUE
C
C     NEW THERMO DATA DATA INPUT IN JANNAF TABLE FORM
C
 3Ø15 DO 1991 I=1,NS
      READ(NUNITB,222) AID(I),WTMOLE(I),HF(I)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,222) AID(I),WTMOLE(I),HF(I)
      DO 1Ø IT=1, NT,2
      ITP1=IT+1
```

```
      READ(NUNITB,1Ø2) TTB(IT,I),  CPTB(I,IT),GTB(I,IT),HTB(I,IT),
     *TTB(ITP1,I),CPTB(I,ITP1),GTB(I,ITP1),HTB(I,ITP1)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,1Ø2)TTB(IT,I),CPTB(I,IT),GTB(I,IT),
     *HTB(I,IT),TTB(ITP1,I),CPTB(I,ITP1),GTB(I,ITP1),HTB(I,ITP1)
      GTB(I,IT)= -GTB(I,IT)*TTB(IT,I)  +HF(I) *1ØØØ.
      GTB(I,ITP1)= -GTB(I,ITP1)*TTB(ITP1,I)  +HF(I)*1ØØØ.
      HTB(I,IT)=(HTB(I,IT)+HF(I))*1ØØØ.
      HTB(I,ITP1)=(HTB(I,ITP1)+ HF(I))*1ØØØ.
   1Ø CONTINUE
      IF(WTMOLE(I)-1.Ø) 1972,1991,1991
 1972 IECC=I
 1991 CONTINUE
C
C     MODIFICATIONS FOR LAPP/ARC INTERFACE PROGRAM
C
      WRITE(NUNITD,333) (TITLE(I),I=1,1Ø)
C
C     IDENTIFY LAPP SPECIES IN THE ARCTABLE
C
C     TABLE=SPECIES NAMES AS FOUND IN ARCTABLE
C     15=NUMBER OF SPECIES IN ARCTABLE
C     IZSPEC=NUMBER OF LAPP SPECIES FOUND IN ARCTABLE
C
      M=Ø
      DO 3 I=1,NS
      DO 3 J=1,16
      IF(AID(I).NE.TABLE(J)) GO TO 3
      M=M+1
      ZSPEC(M)=AID(I)
      ISPEC(M)=I
    3 CONTINUE
      IZSPEC=M
      WRITE(NUNITD,334) IZSPEC
  334 FORMAT(8I1Ø)
      WRITE(NUNITD,333) (ZSPEC(M),M=1,IZSPEC)
      WRITE (NUNITD,1Ø2) THOT,TCOOL
      WRITE(NUNITD,1ØØØ) RJ
      DO 3Ø1 J = 1,6
      DO 3Ø1 I = 1,NS
      IF(AID(I).EQ.XAME(J)) ISAVE(J) = I
  3Ø1 CONTINUE
      DO 1992 I=1,NR
      READ  (NUNITB,444)(ZID(J),J=1,5),IRR(I),IRT(I),(RC(I,K),K=1,3)
      IF(NUNITM.LT.Ø) WRITE(NNOUT,444)(ZID(J),J=1,5),IRR(I),IRT(I),
     *(RC(I,K),K=1,3)
      DO 1993 J=1,5
      IRRR(I,J)=Ø
      DO 1993 L=1,NS
      IF(ZID(J)-AID(L)) 1993,1994,1993
 1994 IRRR(I,J)=L
 1993 CONTINUE
 1992 CONTINUE
      DO 912 I=1,MPSI
      WTVR=Ø.Ø
      DO 632 J=1,NS
```

```
  632 WTVR=WTVR+ALPHA(J,I)*WTMOLE(J)
      DO 633 J=1,NS
  633 ALPHA(J,I)=ALPHA(J,I)/WTVR
  912 CONTINUE
      IF(DELPSI) 9Ø3,3Ø41,9Ø3
 3Ø41 DUM=Ø.Ø
      DO 5ØØ1 J=1,NS
 5ØØ1 DUM=DUM+ALPHA(J,1)
      XMD=MMOD-1
      DELPSI=SQRT(P*U(1)/42.285EØ/T(1)/DUM)*RJ/XMD
  9Ø3 DO 2Ø I=1,29
      XI=I-1
      PSI(I)=XI*DELPSI
      XLE(I)=XLE(1)
   2Ø SIGMA(I)=SIGMA(1)
      DO 9Ø I=NPSI,29
      RT(I)=T(MPSI)
      T(I)=T(MPSI)
      DO 8Ø J=1,NS
      RALPHA(J,I)=ALPHA(J,MPSI)
   8Ø ALPHA(J,I)=ALPHA(J,MPSI)
      RU(I)=U(MPSI)
   9Ø U(I)=U(MPSI)
      IF(NOUT.GT.Ø)CALL INOUT
      PPUNCH = P
      P=2117.Ø*P
      DPDX=Ø.Ø
C
C      PRESSURE OPTION,  IF IPRESS= Ø,  PRESSURE
C         IS CONSTANT AND = TO P, IF IPRESS = 1, COEFFICIENTS CALLED
C         PC(1),PC(2),PC(3),PC(4) ARE INPUT.
C         EQUATION USED IS P = PC(1) + PC(2)*X + PC(3)*X*X + PC(4)*X*X*X
C
    2 IF(IPRESS) 821,822,821
  821 P=(PC(1)+X*(PC(2)+X*(PC(3)+X*PC(4))))*2117.Ø
      DPDX=(PC(2)+X*(2.Ø*PC(3)+X*3.Ø*PC(4)))*2117.Ø
      PPUNCH = P/2117.Ø
  822 DO 31 I=1,MPSI
      WTMIX(I)=Ø.Ø
      DO 3Ø J=1,NS
   3Ø WTMIX(I)=WTMIX(I)+ALPHA(J,I)
      RHO(I)=P/89517.5Ø1/T(I)/WTMIX(I)
   31 RHOOUT(I)=RHO(I)/1.94
      DO 8Ø5 I=1,MPSI
C
C     FREE STREAM VELOCITY WILL BE SET TO 1.Ø FPS IF ZERO IS ENTERED
C
      U(I) = AMAX1(1.ØEØ,U(I))
      TFDG(I)=AMAX1(T(I),1ØØ.ØØEØ)
      T4(I)=TFDG(I)**4
      XLT(I)=ALOG(TFDG(I))
      CPBAR(I)=Ø.Ø
      HSTAT(I)=Ø.Ø
      TX=T(I)
      DO 8Ø5 J=1,NS
```

```
      JJ=J
      CALL TKEY (TX,TTB,ITKEY,SDT,HDT,NT,JJ)
      IF (ITKEY.EQ.Ø) GO TO 9
      CP(J,I)=Ø.Ø
      H(J,I)=Ø.Ø
      CALL LIPLN(ITKEY,J,CPTB,SDT,HDT,AX)
      CP(J,I)=AX*45Ø55.31
      CALL LIPLN(ITKEY,J, HTB,SDT,HDT,AX)
      H(J,I)=AX*45Ø55.31
      HSTAT(I)=HSTAT(I)+H(J,I)*ALPHA(J,I)
  8Ø5 CPBAR(I)=CPBAR(I)+CP(J,I)*ALPHA(J,I)
      ETA(1)=Ø.Ø
      Y(1)=Ø.Ø
C********CALL
      ETA(2)=DELPSI/SQRT(RHO(1)*U(2))
      Y(2)=DELPSI/SQRT(RHO(2)*U(2))
      DO 25 I=3,MPSI
      ETA(I)=SQRT(ETA(I-2)**2+DELPSI*(PSI(I)/U(I)+4.ØEØ*PSI(I-1)/U(I-1)
     1+PSI(I-2)/U(I-2))/1.5/RHO(1))
      TEMP = (Y(I-2)**2+DELPSI*(PSI(I)/RHO(I)/U(I)+4.Ø*PSI(I-1)/RHO(I-1)
     1    /U(I-1)+PSI(I-2)/RHO(I-2)/U(I-2))/1.5)
 1ØØ3 FORMAT(I5,7E1Ø.3)
      IF(TEMP.LT.Ø.Ø) CALL OUTPUT
      Y(I) =SQRT(TEMP)
   25 CONTINUE
C
C**** HAS MIXING REGION INTERSECTED X AXIS YET, YES IF Ø OR -
C
      IF (ITURB-6) 8Ø1Ø,8Ø11,8Ø1Ø
 8Ø1Ø IF (U(1) - USUBØ1) 9ØØØ,9ØØØ,9ØØ1
C
C     MODEL 6 COMMON CALCULATIONS
C

 8Ø11 QQ1 = (U(1)+U(MPSI))/2.Ø
      DO 8Ø12 I=2,MPSI
      IF ((QQ1-U(I))*(QQ1-U(I-1))) 8Ø13,8Ø13,8Ø12
 8Ø12 CONTINUE
 8Ø13 QQ2 = (QQ1-U(I-1))/(U(I)-U(I-1))
      QQ1ØØ = Y(I-1)+(Y(I)-Y(I-1))*QQ2
      QQ3Ø = T(I-1)+(T(I)-T(I-1))*QQ2
      QQ3 = CPBAR(I-1)+(CPBAR(I)-CPBAR(I-1))*QQ2
      QQ4 = 1.Ø/(WTMIX(I-1)+(WTMIX(I)-WTMIX(I-1))*QQ2)
      QQ5 = 89517.5Ø1/QQ4
      QQ6 = QQ3/(QQ3-QQ5)
      QQ7 =SQRT(QQ6*QQ5*QQ3Ø)
      QQ3ØØ = QQ1/QQ7
      QQ8 = (ABS(U(1)-U(MPSI)))/2.Ø
      IF (QQ3ØØ-1.2) 8Ø14,8Ø14,8Ø15
 8Ø14 QQ4ØØ =(.Ø468+QQ3ØØ*((QQ3ØØ*(-.Ø46Ø))+.Ø256*(QQ3ØØ*QQ3ØØ)))*XK2
      GO TO 8Ø16
 8Ø15 QQ4ØØ = .Ø248*XK2
 8Ø16 IF ((U(1)-USUBØ1)*(U(1)-U(MPSI))) 8Ø2Ø,8Ø2Ø,88ØØ
 8Ø2Ø IF (USUBØ1-9ØØØ.Ø) 8Ø21,8Ø21,89ØØ
 8Ø21 USUBØ1 = 1ØØØØ.Ø
```

```
      XDUM=X*Ø.3Ø48
      WRITE(NOUT,99ØØ) XDUM
      GO TO 89ØØ
C
C     MODEL 6 BEFORE MIXING ZONE REACHES AXIS
C
 88ØØ QQ9 = Ø.95*   (U(1)-U(MPSI)) + U(MPSI)
      DO 88Ø2 I = 2,MPSI
      IF ((QQ9-U(I))*(QQ9-U(I-1))) 88Ø4,88Ø4,88Ø2
 88Ø2 CONTINUE
 88Ø4 QQ2ØØ = Y(I-1)+(Y(I)-Y(I-1))*(QQ9-U(I-1))/(U(I)-U(I-1))
      QQ1Ø = QQ4ØØ*QQ8*(QQ1ØØ-QQ2ØØ)
      DO 881Ø I = 1,MPSI
 881Ø XMU(I) = QQ1Ø*RHO(I)
      GO TO 98
C
C     MODEL 6 AFTER MIXING ZONE REACHES AXIS
C
 89ØØ QQ11 = QQ4ØØ*QQ1ØØ*QQ8

      DO 891Ø I = 1,MPSI
 891Ø XMU(I) = QQ11*RHO(I)
      QQ2ØØ = Ø.Ø
      GO TO 98
 9ØØØ IQ77 = 9
      USUBØ1 = Ø.Ø
      WRITE(NOUT,99ØØ)X
 9ØØ1 LL = ITURB + IQ77
C
C      EDDY VISCOSITY  MODELS
C
      GO TO (91,99,8666,78,8667,8668,9ØØ3,91,99,45,78,26,33,78),LL
C
C      MODEL 1 BEFORE MIXING ZONE REACHES AXIS
C
 8666 XMU(1)=Ø.ØØ137*(X+1.ØE-Ø5)*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))
      GO TO 37
C
C      MODEL 3 BEFORE MIXING ZONE REACHES AXIS
C
 8667 XMU(1)=Ø.ØØ137*(X+1.ØE-Ø5)*RHO(1)*ABS(U(1)-U(MPSI))
      GO TO 37
C
C      MODEL 4 BEFORE MIXING ZONE REACHES AXIS
C
 8668 XMU(1)=Ø.ØØ137*(X+1.ØE-Ø5)*RHO(MPSI)*ABS(U(1)-U(MPSI))
      GO TO 37
   91 DO 92 I=1,MPSI
C
C     MODEL Ø LAMINAR FLOW
C
   92 XMU(I)=3.Ø5E-8*T(I)**1.5/(T(I)+111.Ø)
      GO TO 98
   45 DUM=.5*(RHO(1)*U(1)+RHO(MPSI)*U(MPSI))
      DO 52 J=1,MPSI
```

```
      I=MPSI-J+1
      IF(RHO(I)*U(I)-DUM) 52,52,51
   52 CONTINUE
C
C     MODEL 1 AFTER MIXING ZONE REACHES AXIS
C
   51 Z=Y(I)+(Y(I)-Y(I+1))*(RHO(I)*U(I)-DUM)/(RHO(I)*U(I)-RHO(I+1)*U(I+1
     1))
      XMU(1)=XK2*Z*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))*Ø.Ø25
      GO TO 37
   99 DO 39 I=1,MPSI
   39 XMU(I)=XK2*Ø.Ø25
      GO TO 98
   78 RD=(U(1)+U(MPSI))/2.Ø
      DO 47 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 48,48,47
   47 CONTINUE
   48 RHALVE=ETA(I-1)+(ETA(I)-ETA(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
      DUMMY=XK2*RHALVE*ABS(U(1)-U(MPSI))*Ø.Ø25
      XMU(1)=DUMMY*RHO(1)
      DO 79 I=2,MPSI
C
C     MODEL 2 BEFORE MIXING ZONE REACHES AXIS
C
   79 XMU(I)=DUMMY*(RHO(1)*ETA(I)/Y(I))**2/RHO(I)
      GO TO 98
C     MODEL 2 AFTER MIXING ZONE REACHES AXIS
   26 RD=(U(1)+U(MPSI))/2.Ø
      DO 27 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 28,28,27
   27 CONTINUE
   28 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
C
C     MODEL 3 AFTER MIXING ZONE REACHES AXIS
C
      XMU(1)=XK2*RHALVE*RHO(1)*ABS(U(1)-U(MPSI))*Ø.Ø25
      DO 29 I=1,MPSI
   29 XMU(I)=XMU(1)
      GO TO 98
   33 RD=(U(1)+U(MPSI))/2.Ø
      DO 34 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 35,35,34
   34 CONTINUE
   35 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
C
C     MODEL 4 AFTER MIXING ZONE REACHES AXIS
C
      XMU(1)=XK2*RHALVE*RHO(MPSI)*ABS(U(1)-U(MPSI))*Ø.Ø25
   37 DO 36 I=1,MPSI
   36 XMU(I)=XMU(1)
      GO TO 98
C
C      MODEL 5 BEFORE MIXING ZONE REACHES AXIS
C
 9ØØ3 XMU(1) = Ø.ØØ137*(X+1.ØE-Ø5)*ABS(UNIT-U(MPSI))*RHO(1)
```

```
      DO 9ØØ4 I = 2,MPSI
      XMU(I)=Ø.ØØ137*(X+1.ØE-Ø5)*ABS(UNIT-U(MPSI))*(RHO(1)**2/RHO(I))
 9ØØ4 CONTINUE
   98 A(1)=Ø.Ø
C
C     CALCULATE A
C
      DO 44 I=2,MPSI
   44 A(I)=XMU(I)*RHO(I)*U(I)*Y(I)*Y(I)/PSI(I)
      DO 899 L=1,NPSI
      RRT=1.986*T(L)
      ROOTT=SQRT(T(L))
      TX=T(L)
      DO 855 I=1,NS
      II=I
      CALL TKEY(TX,TTB,ITKEY,SDT,HDT,NT,II)
      IF (ITKEY.EQ.Ø) GO TO 9
      G(I)=Ø.Ø
      WP(I)=Ø.Ø
      WM(I)=Ø.Ø
      QX(I,L)=Ø.Ø
      DO 872 J=1,NS
  872 CM(I,J,L)=Ø.Ø
      CALL LIPLN(ITKEY,I, GTB,SDT,HDT,AX)
      G(I)=AX
  855 CONTINUE
C
C     REACTION CALCULATION
C     REACTION KINETICS CONTINUE DOWN TO 4ØØ DEGREES K
C        UNLESS TKINET IS SET TO A VALUE OTHER THAN 4ØØ K
C     REACTION KINETICS FOR ALL REACTIONS CONTINUE DOWN TO TKINET
C
      IF(T(L)-TKINET) 3256,3256,3259
 3259 CONTINUE
      DO 862 I=1,NR
      RP(I,L)=Ø.Ø
      RM(I,L)=Ø.Ø
      KK = IRT(I)
C
C     REACTION CONSTANT TYPE
C
      GO TO (841,842,843,844,845,846,847),KK
  841 RATE=RC(I,1)*AV
      GO TO 849
  842 RATE=RC(I,1)/T(L)*AV
      GO TO 849
  843 RATE=RC(I,1)/T(L)/T(L)*AV
      GO TO 849
  844 RATE=RC(I,1)/ROOTT*AV
      GO TO 849
  845 RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV
      GO TO 849
  846 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T(L)**RC(I,2)*AV
      GO TO 849
  847 RATE=RC(I,1)/T(L)/ROOTT*AV
```

```
  849 CONTINUE
      K=IRR(I)
C
C     TYPE OF REACTION
C
      GO TO(864,865,866,87Ø,871,834,835,836,837,838),K
  87Ø J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      E = (G(J1)+G(J2)-G(J3))/RRT
      IF(ABS(E).LT.8Ø.Ø) GO TO 7ØØ
      IF(E.LT.Ø.Ø) E=EXP(-8Ø.ØEØ)
      IF(E.GT.Ø.Ø) E =EXP(8Ø.ØEØ)
      GO TO 7Ø1
7ØØ   E =EXP(E)
7Ø1   CONTINUE
       CRR=RATE*RHOOUT(L)
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)/E/R/T(L)
      DO 771 J=1, 3
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
  771 QX(IROW,L)= QX(IROW,L)+ SIGN*RP(I,L)
      GO TO 868
  871 J1=IRRR(I,1)
      J2=25
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      E = (G(J1)-G(J3)-G(J4))/RRT
      IF(ABS(E).LT.8Ø.Ø) GO TO 7Ø2
      IF( E.LT.Ø.Ø) E =EXP(-8Ø.ØEØ)
      IF( E.GT.Ø.Ø) E =EXP(8Ø.ØEØ)
      GO TO 7Ø3
7Ø2   E =EXP(E)
7Ø3   CONTINUE
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)
      RP(I,L)=CRR*ALPHA(J1,L)
      RM(I,L)=CRR*R*T(L)*RHOOUT(L)*ALPHA(J3,L)*ALPHA(J4,L)/E
      DO 772 J=1, 4
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      IF(J.EQ.2) IROW=25
      CM(IROW,J1,L)= CM(IROW,J1,L)+SIGN*CRR
      CM(IROW,J3,L)= CM(IROW,J3,L)-SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
  772 QX(IROW,L)= QX(IROW,L)- SIGN*RM(I,L)
      GO TO 867
  864 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
```

```
      J4=IRRR(I,4)
      E = (G(J1)+G(J2)-G(J3)-G(J4))/RRT
      IF(ABS(E).LT.8Ø.Ø) GO TO 7Ø4
      IF(E.LT.Ø.Ø) E =EXP(-8Ø.ØEØ)
      IF(E.GT.Ø.Ø) E =EXP(8Ø.ØEØ)
      GO TO 7Ø5
7Ø4   E = EXP(E)
7Ø5   CONTINUE
       CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E
      DO 773 J=1,  4
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
  773 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-RM(I,L))
      GO TO 867
  865 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      E = (G(J1)+G(J2)-G(J3))/RRT
      IF(ABS(E).LT.8Ø.Ø) GO TO 7Ø6
      IF(E.LT.Ø.Ø) E=EXP(-8Ø.ØEØ)
      IF(E.GT.Ø.Ø) E=EXP(8Ø.ØEØ)
      GO TO 7Ø7
7Ø6   E =EXP(E)
7Ø7   CONTINUE
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)/(E*R*T(L))
      DO 774 J=1,3
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
  774 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L  ))
      GO TO 868
  866 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
      E = (G(J1)+G(J2)-G(J3)-G(J4)-G(J5))/RRT
      IF(ABS(E).LT.8Ø.ØEØ) GO TO 7Ø8
      IF(E.LT.Ø.Ø) E=EXP(-8Ø.ØEØ)
      IF(E.GT.Ø.Ø) E =EXP(8Ø.ØEØ)
      GO TO 7Ø9
7Ø8   E =EXP(E)
7Ø9   CONTINUE
```

```
      CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RHOOUT(L)*R*T(L)/E
      DO 775 J=1, 5
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
      CM(IROW,J5,L)= CM(IROW,J5,L)-SIGN*RM(I,L)/ALPHA(J5,L)
  775 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-2.*RM(I,L))
      GO TO 861
  837 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      CRR=RATE*RHOOUT(L)
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=Ø.Ø
      DO 776 J=1, 3
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
  776 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
      GO TO 868
  838 J1=IRRR(I,1)
      J2=25
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)
      RP(I,L)=CRR*ALPHA(J1,L)
      RM(I,L)=Ø.Ø
      DO 777 J=1, 4
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      IF (J.EQ.2) IROW=25
  777 CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*CRR
      GO TO 867
  834 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=Ø.Ø
      DO 778 J=1, 4
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
```

```
  778 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
      GO TO 867
  835 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=Ø.Ø
      DO 779 J=1, 3
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
  779 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
      GO TO 868
  836 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
       CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=Ø.Ø
      DO 78Ø J=1, 5
      SIGN=1.Ø
      IF (J.GT.2) SIGN=-1.Ø
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
  78Ø QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
C
C     CALCULATE WDOT
C
  861 WP(J5)=WP(J5)+RP(I,L)
      WM(J5)=WM(J5)+RM(I,L)
  867 WP(J4)=WP(J4)+RP(I,L)
      WM(J4)=WM(J4)+RM(I,L)
  868 WP(J3)=WP(J3)+RP(I,L)
      WM(J3)=WM(J3)+RM(I,L)
      WP(J2)=WP(J2)+RM(I,L)
      WM(J2)=WM(J2)+RP(I,L)
      WP(J1)=WP(J1)+RM(I,L)
      WM(J1)=WM(J1)+RP(I,L)
  862 CONTINUE
 3256 CONTINUE
      DO 897 J=1,NS
  897 WDOT(J,L)=(WP(J)-WM(J))/RHOOUT(L)/U(L)
  899 CONTINUE
      IOUT=IOUT+1
   63 IF(IFINIS) 65,69,65
   65 IF(X-XMAX) 67,66,66
   67 IF(PRNT-PCNT) 69,69,68
   68 CONTINUE
      GO TO 5
```

```
   66 IFINIS=2
   69 CALL OUTPUT
      PCNT=Ø.Ø
      IF(IFINIS-1) 5,5,6
C
C       CHECK DIFFUSION STEP SIZE
C
    5 XD=DELPSI*DELPSI*SIGMA(1)/XMU(1)/XLE(1)/12.Ø *FDL
      DO 511 I=2,NPSI
      DUMMY=A(I+1)+A(I-1)+A(I)+A(I)
      DUMMY=PSI(I)*DELPSI*DELPSI*SIGMA(I)/XLE(I)/DUMMY/1.5*FDL
  511 XD=AMIN1(XD,DUMMY)
      DX=AMIN1(DX,XD)
      DO 1Ø1 I=2,NPSI
      EX1=PSI(I)*DELPSI**2/DX
      EX11=.5*(A(I)+A(I+1))
      EX12=.5*(A(I)+A(I-1))
C
C     INTEGRATE MOMENTUM EQUATION
C
      RU(I)=(EX11*(U(I+1)-U(I))+EX12*(U(I-1)-U(I)))/EX1+U(I)
      RU(I)=RU(I)-DX*DPDX/RHO(I)/U(I)
      EX3=Ø.Ø
      EX4=Ø.Ø
      DO 21 J=1,NS
      EX3=EX3+H(J,I)*WDOT(J,I)
   21 EX4=EX4+CP(J,I)*(ALPHA(J,I+1)-ALPHA(J,I-1))
      EX2=EX1*CPBAR(I)
      EX5=XLE(I)*A(I)/SIGMA(I)
      EX6=.5*(EX5+XLE(I+1)*A(I+1)/SIGMA(I+1))
      EX7=.5*(EX5+XLE(I-1)*A(I-1)/SIGMA(I-1))
      EX8=CPBAR(I)*A(I)/SIGMA(I)
      EX9=.5*(EX8+CPBAR(I+1)*A(I+1)/SIGMA(I+1))
      EX1Ø=.5*(EX8+CPBAR(I-1)*A(I-1)/SIGMA(I-1))
      EX14=EX4*EX5/4.Ø
C
C     INTEGRATE ENERGY EQUATION
C
      RT(I)=(U(I+1)-U(I-1))**2*A(I)/EX2/4.Ø+DX*DPDX/RHO(I)/CPBAR(I)+T(I)
     1+((EX9+EX14)*T(I+1)+(EX1Ø-EX14)*T(I-1)-(EX9+EX1Ø)*T(I))/EX2-EX3*DX
     2/CPBAR(I)
      RHOUIX=DX/(RHOOUT(I)* U(I))
C
C     INTEGRATE SPECIES EQUATIONS
C
      DO 41 J=1,NS
   41 QX1(J)      =(EX6*(ALPHA(J,I+1)-ALPHA(J,I))+EX7*(ALPHA(J,I-1)-ALPHA
     1(J,I)))/EX1+ALPHA(J,I)+  QX(J,I)*RHOUIX
      DO 781 M=1,NS
      DO 781 N=1,NS
      CM1(M,N)= CM(M,N,I)*RHOUIX
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.Ø
  781 CONTINUE
      CALL SLDP(QX1,CM1,NS)
  785 FORMAT (1H , 2I5)
```

```
      DO 782 J=1, NS
  782 RALPHA(J,I)= QX1(J)
  1Ø1 CONTINUE
      EX3=4.Ø*XMU(1)*DX/DELPSI/DELPSI
      RHOUIX=DX/(RHOOUT(1)* U(1))
C
C     COMPUTE U AT CENTER LINE
C
      RU(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)
      EX4=Ø.Ø
      DO 2ØØ J=1,NS
      EX4=EX4+H(J,1)*WDOT(J,1)
      RALPHA(J,MPSI)=ALPHA(J,MPSI)
  2ØØ QX1(J)      =EX3*XLE(1)*(ALPHA(J,2)-ALPHA(J,1))/SIGMA(1)+ALPHA(J,1)
     1+  QX(J,1)*RHOUIX
      DO 783 M=1,NS
      DO 783 N=1,NS
      CM1(M,N)= CM(M,N,1)*RHOUIX
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.Ø
  783 CONTINUE
      CALL SLDP(QX1,CM1,NS)
      DO 784 J=1, NS
C
C     COMPUTE SPECIES AT CENTER LINE
C
  784 RALPHA(J,1)= QX1(J)
C
C     CALCULATE TEMP. AT CENTER LINE
C
      RT(1)=EX3*(T(2)-T(1))/SIGMA(1)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)
     1-EX4*DX/CPBAR(1)
      RT(MPSI)=T(MPSI)
      IF(IEDGE) 23Ø,231,23Ø
C
C     COMPUTE TEMP. AND U AT EDGE
C
  23Ø RU(MPSI)=U(MPSI)-DX*DPDX/RHO(MPSI)/U(MPSI)
      RT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)
      DO 21Ø I=MPSI,29
      RU(I)=RU(MPSI)
      U(I)=RU(MPSI)
      RT(I)=RT(MPSI)
  21Ø T(I)=RT(MPSI)
  231 CONTINUE
    1 IFINIS=1
  921 SAVEX=X
      SAVEDX=DX
      DO 941 I=1,29
      SAVEU(I)=U(I)
      SAVET(I)=T(I)
      DO 94Ø J=1,NS
      SAVEA(J,I)=ALPHA(J,I)
  94Ø CONTINUE
  941 CONTINUE
      MINIT = 13
```

```
      MHALF = 25
      NTEST=MPSI-1
      DO 967 I=1,NTEST
C
C      CHECK NEGATIVE MOLE FRACTION
C
  965 DO 967 J=1,NS
      IF (RALPHA(J,I)) 995,967,967
  967 CONTINUE
      X=X+DX
      PCNT=PCNT+DX
      DX=XD
      DO 925 I=1,29
      DO 926 J=1,NS
  926 ALPHA(J,I)=RALPHA(J,I)
      T(I)=RT(I)
  925 U(I)=RU(I)
      GO TO 999
  995 IF (DX.LT.DXMIN)  GO TO 8ØØØ
  981 DX=SAVEDX/2.Ø
      X=SAVEX
      DO 985 I=1,29
      DO 982 J=1,NS
  982 ALPHA(J,I)=SAVEA(J,I)
      T(I)=SAVET(I)
  985 U(I)=SAVEU(I)
      GO TO 2
C
C     IF MPSI .GE.26 ,MPSI IS HALVED
C
  999 IF(MPSI-MHALF) 1ØØ1,15ØØ,15ØØ
 1ØØ1 IF(ABS(U(NPSI)-U(MPSI))/U(MPSI)-.Ø1ØEØ) 1Ø11,1Ø11,1ØØ4
 1Ø11 IF(ABS(T(NPSI)-T(MPSI))/T(MPSI)-.Ø5ØEØ) 1ØØ2,1ØØ2,1ØØ4
 1ØØ2 CONTINUE
      GO TO 2ØØØ
 1ØØ4 MPSI=MPSI+1
      NPSI=MPSI-1
      DO 11Ø1 I=MPSI,29
      SAVEU(I)=U(NPSI)
      RU(I)=U(NPSI)
      U(I)=U(NPSI)
      SAVET(I)=T(NPSI)
      T(I)=T(NPSI)
      RT(I)=T(NPSI)
      DO 11Ø2 J=1,NS
      SAVEA(J,I)=ALPHA(J,NPSI)
      ALPHA(J,I)=ALPHA(J,NPSI)
 11Ø2 RALPHA(J,I)=ALPHA(J,NPSI)
 11Ø1 CONTINUE
      GO TO 2ØØØ
 15ØØ IFINIS=Ø
      DELPSI=DELPSI+DELPSI
      DO 16ØØ I=1,MINIT
      DO 165Ø J=1,NS
 165Ø ALPHA(J,I)=ALPHA(J,2*I-1)
```

```
      T(I)=T(2*I-1)
 1600 U(I)=U(2*I-1)
      MPSI=MINIT
      NPSI=MPSI-1
      DO 1700 I=MINIT,29
      DO 1750 J=1,NS
      ALPHA(J,I)=ALPHA(J,MPSI)
 1750 RALPHA(J,I)=ALPHA(J,MPSI)
      T(I)=T(MPSI)
      RT(I)=T(MPSI)
      U(I)=U(MPSI)
 1700 RU(I)=U(MPSI)
      DO 1800 I=2,29
 1800 PSI(I)=PSI(I-1)+DELPSI
      ITER=0
      ISTEP=0
      GO TO 2000
 8000 WRITE(NDBG,8001)
 8001 FORMAT(68H1NEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING
     1OF STEP SIZE)
      IFINIS=2
      GO TO 69
 2000 CONTINUE
      CALL TICK(ISECS)
      IELAPS = ISECS-ISECST
      IF(IELAPS.LT.0) IELAPS = IDIFFT + ISECS
      IF(IELAPS.GE.ILIMIT) GO TO 6
      GO TO 2
  100 FORMAT(14I5)
  102 FORMAT(8F10.4)
  111 FORMAT (7(  E10.3))
  222 FORMAT(A6,7E10.3)
  333 FORMAT(10A8)
  444 FORMAT(A6,1X,A6,8X,A6,1X,A6,1X,A6,7X,I2,I1,E8.2,F4.1,F9.1)
  555 FORMAT(8(  E10.3))
  666 FORMAT(10I5)
 1000 FORMAT(7E10.3)
 9900 FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X =   E15.7)
    6 CONTINUE
      XORJ=X/RJ
  790 FORMAT(  E10.3,60X,E10.3)
      IF (IPUNCH .EQ. 0 .OR. IPUNCH .EQ. 1)  GO TO 9
      X=X*AMULT
      XMAX=XMAX*AMULT
      PRNT=PRNT*AMULT
      RJ=RJ*AMULT
      DXMIN=DXMIN*AMULT
      PC(2)=PC(2)/AMULT
      PC(3)=PC(3)/AMULT1
      PC(4)=PC(4)/AMULT2
      DELPSI=DELPSI*AMULT3
      DO 7666 I=1,MPSI
 7666 U(I)=U(I)*AMULT
      WRITE(NUNITE,333)(TITLE(I),I=1,10)
      WRITE(NUNITE,666)MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,
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     *IPRESS,NT
      WRITE(NUNITE,1000)FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),
     *FREQA(6)
      WRITE(NUNITE,1000) X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2
      WRITE(NUNITE,1000)  DXMIN, FDL,    PC(1),PC(2),PC(3),PC(4)
      WRITE(NUNITE,1000) PPUNCH,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET
      WRITE(NUNITE,1000) (T(I),I=1,MPSI)
      WRITE(NUNITE,1000) (U(I),I=1,MPSI)
      DO 8 I = 1,MPSI
      DO 1104 J=1,NS
 1104 RALPHA(J,I)=RALPHA(J,I)/WTMIX(I)
      WRITE(NUNITE,1000) (RALPHA(J,I),J=1,NS)
    8 CONTINUE
    9 CONTINUE
      STOP
      END
      SUBROUTINE OUTPUT
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
     2           WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),
     3RU(30),U(30),TITLE(12),XLE(30),XMU(30)           ,G(25),WTMIX(30),
     4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),
     5          IRR(49),FREQ(30),SAVEA(25,30),              PC(4),ZID(5),
     6          ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),
     7T4(30),TFDG(30),IRT(49),RP(49,30),RM(49,30)
      DIMENSION ISAVE(6), FREQA(6), ALOC(50,6), ATT(6), YATT(50)
      DIMENSION ZCON(16,30)
      COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
      COMMON/UNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,
     *NUNITG,NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NUNITN,
     *NOUT,NDBG,NNNOUT
      COMMON/C/ IZSPEC,ISPEC(16)
      COMMON  A      , RHO    , Y      , T      , PSI    , RT
      COMMON  SUM    , AR     , HSTAT  , H      , ALPHA  , RALPHA
      COMMON  CP     , SIGMA           , WTMOLE , CPBAR  , C
      COMMON  AID    , ETA    , RATIO  , RU     , U      , TITLE
      COMMON  XLE    , XMU    ,          G      , WTMIX  , WDOT
      COMMON  SAVEU  , SAVET  , WM     , WP     , RC
      COMMON           SAVEA  ,          PC     , X      , XMAX
      COMMON  PRNT   , DXMIN  , DX     , FDL    , DELPSI , RJ
      COMMON  XK2    , P      , ZID    , FREQ   , ECC    , DPDX
      COMMON  Y   OUT   , HOUT   , RHOOUT , IRRR   , IRR    , IFINIS
      COMMON  IPAGE  , MPSI   , MY     , NS     , NR     , IEDGE
      COMMON  ITURB  , IPRESS , NPSI   , ITEST  , ITER   , IECC
      COMMON  IRT    , XMU  OUT , XLT    , T4     , TFDG   , IOUT
      COMMON  IOUT1  , IOUT2  ,RP      , RM     , ISAVE  , IPUNCH
      COMMON TKINET,NFREQA,ALOC,FREQA,QQ100,QQ200,QQ300,QQ400
      DATA AMULT5/1000./,AMULT4/1.488/
      DATA BLANK/8H        /
      DATA ZCO /6HCO    /
      DATA ZCO2/6HCO2   /
      DATA ZH2O/6HH2O   /
      DATA ZO  /6HO     /
      DATA ZOH/6HOH    /
      DATA ZAL/6HAL2O3 /
```

```
      DUMMY = Ø.Ø
      BIG=1.ØE3Ø
      NS1=NS+1
      IF(NS1 .GT. 25) GO TO 2
      DO 1 I=NS1,25
1     AID(I)=BLANK
2     DO 5 I=1, NS
      IF (AID(I).EQ.ZCO )  ICO =I
      IF (AID(I).EQ.ZCO2)  ICO2=I
      IF (AID(I).EQ.ZH2O)  IH2O=I
      IF (AID(I).EQ.ZO  )  IO  =I
      IF (AID(I).EQ.ZOH) IOH=I
      IF (AID(I).EQ.ZAL) IAL=I
    5 CONTINUE
      IF(IECC) 531,539,531
  531 DO 532 I=1,MPSI
  532 ECC(I)=RHO(I)*ALPHA(IECC,I)*3.1Ø8E23
  539 DO 1Ø I=1,MPSI
      YOUT(I)=Y(I)/RJ
      XMUOUT(I)=XMU(I)*32.174
      HOUT(I)=HSTAT(I)/45Ø55.31
      SUM(I)=Ø.Ø
      DO 1Ø J=1,NS
   1Ø SUM(I)=SUM(I)+ALPHA(J,I)*WTMOLE(J)
      UD=.Ø5*U(1)+.95*U(MPSI)
      DO 83 I=2,MPSI
      IF ((U(I)-UD)*(U(I-1)-UD)) 84,84,83
   83 CONTINUE
   84 VR=(Y(I)-Y(I-1))*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)
      TD=.Ø5*T(1)+.95*T(MPSI)
      DO 85 I=2,MPSI
      IF ((T(I)-TD)*(T(I-1)-TD)) 86,86,85
   85 CONTINUE
   86 TR=(Y(I)-Y(I-1))*(TD-T(I-1))/(T(I)-T(I-1))+Y(I-1)
      TR=TR/RJ
      VR=VR/RJ
      DO 87 J=1,NS
      AR(J)=Ø.Ø
      AD=.Ø5*ALPHA(J,1)+.95*ALPHA(J,MPSI)
      IF(ALPHA(J,MPSI)) 91,92,91
   91 DO 88 I=1,MPSI
      IF(ALPHA(J,I)-AD) 88,88,89
   88 CONTINUE
   89 AR(J)=Y(I-1)+(Y(I)-Y(I-1))*(AD-ALPHA(J,I-1))/(ALPHA(J,I)-ALPHA(J,I
     1-1))
      AR(J)=AR(J)/RJ
      GO TO 87
   92 DO 93 I=1,MPSI
      IF(ALPHA(J,I)-AD) 94,93,93
   93 CONTINUE
   94 GO TO 89
   87 CONTINUE
      PCNT=Ø.Ø
      IPAGE=IPAGE+1
      XXOUT=X*AMULT
```

```
      XXX=XXOUT
      WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
      WRITE (NOUT,102)
      XORJ=X/RJ
      POUT=P/2117.0
      DPOUT=DPDX/2117.0
      DDX=DX*AMULT
      WRITE(NOUT,103) XORJ,DDX,POUT
      IF (ITURB-6) 8600,8500,8600
 8500 WRITE (NOUT,8555)
      QQ101=QQ100/RJ
      QQ201=QQ200/RJ
      WRITE (NOUT,8556) QQ101,QQ201,QQ300,QQ400
 8555 FORMAT(1H0,8X,4HHALF,21X,12HINNER MIXING,17X,11HMACH NUMBER,16X,11
     *HMIXING RATE/7X,10HRADIUS/R  ,16X,15HZONE RADIUS/R  ,14X,14HAT HAL
     *F RADIUS,14X,11HCOEFFICIENT)
 8556 FORMAT (4X,  E14.6,  3E28.6)
 8600 WRITE (NOUT,107)
      WRITE (NOUT,509)
      TTT=T(1)
      WRITE(NNNOUT,8888)XXX,TTT
 8888 FORMAT(F6.1,F8.1)
      DO 73 I=1,MPSI
      SS1= 89517.501*WTMIX(I)
      SS2= CPBAR(I)/(CPBAR(I)-SS1)
      SS=SQRT(SS2*SS1*T(I))
      XMACH= U(I)/SS
      UU=U(I)*AMULT
      RRHOUT=RHOOUT(I)*AMULT5
      XXMOUT=XMUOUT(I)*AMULT4
      PPSI=PSI(I)*AMULT3
      IF(IECC) 71,72,71
   71 WRITE (NOUT,207)I,YOUT(I),UU,T(I),RRHOUT,XMACH, HOUT(I),
     *XXMOUT,ECC(I),PPSI,I
      GO TO 73
   72 WRITE (NOUT,307)I,YOUT(I),UU,T(I),RRHOUT,XMACH, HOUT(I),
     *XXMOUT,PPSI,I
   73 CONTINUE
      DO 581  I=1,MPSI
      DO 581  J=1,NS
  581 RALPHA(J,I)=ALPHA(J,I)/WTMIX(I)
      IRPT=(NS+6)/7
      DO 564 KK=1,IRPT
      I1=1+(KK-1)*7
      I2=7+(KK-1)*7
      WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
      WRITE (NOUT,409)
      IF (I2.GE.25) GO TO 50
      WRITE (NOUT,108)(AID(J),J=I1,I2)
      DO 81 I=1,MPSI
   81 WRITE (NOUT,208)I,YOUT(I),(RALPHA(J,I),J=I1,I2),I
      IF(IOUT1)564,564,74
   74 WRITE (NOUT,420)
      WRITE (NOUT,421)(AID(J),J=I1,I2)
      DO 82 I=1,MPSI
```

```
      IF(T(I)-TKINET) 564,564,82
   82 WRITE (NOUT,422)I,(WDOT(J,I),J=I1,I2),I
      GO TO 564
50    I2=25
      WRITE (NOUT,108) (AID(J),J=I1,I2)
      DO 52 I=1,MPSI
   52 WRITE (NOUT,53) I,YOUT(I),(RALPHA(J,I),J=I1,I2),I
53    FORMAT (I3,F9.5,4E13.5,42X,I3)
      IF (IOUT1) 564,564,54
54    WRITE (NOUT,420)
      WRITE (NOUT,55) (AID(J),J=I1,I2)
55    FORMAT (3H0PT,8X,4(3X,A6,4X),43X,3H PT)
      DO 56 I=1,MPSI
      IF (T(I)-TKINET) 564,564,56
56    WRITE (NOUT,57) I,(WDOT(J,I),J=I1,I2),I
57    FORMAT (I3,9X,4E13.5,42X,I3)
564   CONTINUE
      IF(IOUT2)567,567,75
   75 IRPT=(NR+9)/10
      N=0
      NNR=NR-1
      DO 565 KK=1,IRPT
      LL=0
      N=N+1
      WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
   65 I1=1+(N-1)*5
      I2=5+(N-1)*5
      NNN1=I1
      NNN2=I1+1
      NNN3=I1+2
      NNN4=I1+3
      NNN5=I2
      WRITE(NOUT,209)
      WRITE (NOUT,431)NNN1,NNN2,NNN3,NNN4,NNN5
      WRITE (NOUT,432)
      DO 63 I=1,MPSI
      IF(T(I)-TKINET) 566,566,63
   63 WRITE(NOUT,433)I,YOUT(I),(RP(J,I),RM(J,I),J=I1,I2),I
  566 IF(NNR/(5*N))565,565,64
   64 IF(LL)565,66,565
   66 N=N+1
      LL=1
      GO TO 65
  565 CONTINUE
  567 CONTINUE
568   CONTINUE
 1065 CONTINUE
      WRITE (NOUT,1068)
 1066 DO 602 I=1,NPSI
      FT1 = 1.0/SQRT(T(I))
      FT2 = 1.0/FT1
      FT3 = 1.0/T(I)
      FT4 = T(I)**0.75
      SUMS = 0.0
      DO 603 IDX = 1,6
```

```
      IF(ISAVE(IDX).EQ.Ø) GO TO 6Ø3
      K = ISAVE(IDX)
      TERM = RALPHA(K,I)
      GO TO (6Ø4,6Ø5,6Ø6,6Ø7,6Ø8,614),IDX
  6Ø4 Q = (1.29E-17)*FT2 + 2.46E-16
      GO TO 6Ø9
  6Ø5 Q = (Ø.758E-13)*FT1
      GO TO 6Ø9
  6Ø6 Q = (1.53E-11)*FT3
      GO TO 6Ø9
  6Ø7 Q = (9.ØE-18)*FT2 + 8.9E-16
      GO TO 6Ø9
  6Ø8 Q = 3.29E-23*6.21E5*FT2
      GO TO 6Ø9
  614 Q= 1.85*(6.21)**(-2)*(1.ØE-1Ø)*FT3
  6Ø9 SUMS = SUMS + Q*TERM
  6Ø3 CONTINUE
      XNEU = (4.57E27)*SUMS*POUT*FT1
      ECON= Ø.Ø7157*   ECC(I)/XNEU/.Ø254
  6Ø2 IF(IZSPEC.EQ.Ø) GO TO 613
      WRITE(NUNITD,786) XORJ,MPSI
      DO 615 I=1,MPSI
      YY=Y(I)/RJ
      PP=P/2117.Ø
      WRITE(NUNITD,785) YY,T(I),PP
      DO 616 M=1,IZSPEC
      K=ISPEC(M)
  616 ZCON(M,I)=RALPHA(K,I)
      LINES=IZSPEC/7+1.1
      IF(IZSPEC.EQ.7) LINES=1
      DO 559 L=1,LINES
      LSTART=(L-1)*7+1
      LEND=MINØ(IZSPEC,L*7)
  559 WRITE(NUNITD,785) (ZCON(K,I),K=LSTART,LEND)
  615 CONTINUE
  613 CONTINUE
  1Ø2 FORMAT(/,8X,3HX/R,8X,14HDELTA X METERS,4X,1ØHPRESS(ATM))
  1Ø3 FORMAT(4X,  6E14.6)
  1Ø7 FORMAT(4HØ PT,5X,3HY/R, 6X,8HVELOCITY,4X,11HTEMPERATURE,5X,7HDENSI
     1TY, 4X8HMACH NO. , 8X,8HENTHALPY,5X,9HVISCOSITY,
     2 8X,3HPSI,12X,2HPT )
  1Ø8 FORMAT(1Ø3X,3H PT,T1,3HØPT,3X,5H Y/R ,7(3X,A8,2X))
  2Ø1 FORMAT(1H1,//////3H X=  E15.7,7H METERS,8X,1ØA8,8X,4HPAGEI4)
  2Ø7 FORMAT(I4,F1Ø.4,  8E14.6,I4)
  2Ø8 FORMAT(I3,F9.5,  7E13.5,I3)
  2Ø9 FORMAT(1H ,//4ØX,28HREACTION RATES (MOLE/ML-SEC)//)
  3Ø7 FORMAT(I4,F1Ø.4,  7E14.6,4X,I4)
  4Ø9 FORMAT(1HØ,44X,14HMOLE FRACTIONS)
  42Ø FORMAT(1HØ,35X,36HNET RATE OF PRODUCTION (W-DOT/RHO*U))
  421 FORMAT(3HØPT,8X,7(3X,A6,4X),1X,3H PT)
  422 FORMAT(I3,9X,  7E13.5,I3)
  431 FORMAT(1HØ,2HPT,4X,3HY/R, 8X,5(8HREACTION,I3,11X),2HPT)
  432 FORMAT(19X,5(2HRP, 9X,2HRM,1ØX))
  433 FORMAT(I3,1X,  11E11.4,I4)
  5Ø9 FORMAT(18X,1ØHMETERS/SEC,4X,1ØH    K     ,6X,5HGM/CC,22X,6HCAL/GM,
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```
     *7X,8HKG/M/SEC)
 61Ø FORMAT(3X,I3,5X,F7.3,8(2X,  E1Ø.4))
 611 FORMAT(3E15.7)
 612 FORMAT(E15.7,I5)
 78Ø FORMAT(8(  E1Ø.3))
 785 FORMAT(1ØX,7E1Ø.3)
 786 FORMAT(E1Ø.3,I1Ø)
 79Ø FORMAT(  E1Ø.3,6ØX,E1Ø.3)
1Ø68 FORMAT (1HØ)
     RETURN
     END
     SUBROUTINE INOUT
     DIMENSION A(3Ø),RHO(3Ø),Y(3Ø),T(3Ø),PSI(3Ø),RT(3Ø),SUM(3Ø),AR(25),
    1HSTAT(3Ø),H(25,3Ø),ALPHA(25,3Ø),RALPHA(25,3Ø),CP(25,3Ø),SIGMA(3Ø),
    2           WTMOLE(25),CPBAR(3Ø),C(25,9),AID(25),ETA(3Ø),RATIO(3Ø),
    3RU(3Ø),U(3Ø),TITLE(12),XLE(3Ø),XMU(3Ø)              ,G(25),WTMIX(3Ø),
    4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,3Ø),SAVET(3Ø),SAVEU(3Ø),
    5           IRR(49),FREQ(3Ø),SAVEA(25,3Ø),                PC(4),ZID(5),
    6           ECC(3Ø),HOUT(3Ø),YOUT(3Ø),RHOOUT(3Ø),XMUOUT(3Ø),XLT(3Ø),
    7T4(3Ø),TFDG(3Ø),IRT(49),RP(49,3Ø),RM(49,3Ø)
     DIMENSION ISAVE(6)
     COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
     COMMON/UNITS/ NNDUM(14),ND,NDBG
     COMMON  A      , RHO     , Y      , T      , PSI    , RT
     COMMON  SUM    , AR      , HSTAT  , H      , ALPHA  , RALPHA
     COMMON  CP     , SIGMA            , WTMOLE , CPBAR  , C
     COMMON  AID    , ETA     , RATIO  , RU     , U      , TITLE
     COMMON  XLE    , XMU     ,          G      , WTMIX  , WDOT
     COMMON  SAVEU  , SAVET   , WM     , WP     , RC
     COMMON           SAVEA   ,          PC     , X      , XMAX
     COMMON  PRNT   , DXMIN   , DX     , FDL    , DELPSI , RJ
     COMMON  XK2    , P       , ZID    , FREQ   , ECC    , DPDX
     COMMON  YOUT   , HOUT    , RHOOUT , IRRR   , IRR    , IF   INIS
     COMMON  IPAGE  , MPSI    , MY     , NS     , NR     , IEDGE
     COMMON  ITURB  , IPRESS  , NPSI   , ITEST  , ITER   , IECC
     COMMON  IRT    , XMUOUT  , XLT    , T4     , TFDG   , IOUT
     COMMON  IOUT1  , IOUT2   ,RP      , RM     , ISAVE  , IPUNCH
     COMMON TKINET
C
     X=X*AMULT
     XMAX=XMAX*AMULT
     PRNT=PRNT*AMULT
     RJ=RJ*AMULT
     DXMIN=DXMIN*AMULT
     DO 7666 I=1,MPSI
7666 U(I)=U(I)*AMULT
C
     WRITE(ND,19Ø1)
     WRITE(ND,19Ø2)
     WRITE(ND,19Ø3)(TITLE(I),I=1,1Ø)
     IF(IPRESS.NE.Ø) WRITE(ND,19Ø4)P
     IF(IPRESS.EQ.Ø) WRITE(ND,19Ø5)P
     WRITE(ND,19Ø8)RJ
     WRITE(ND,19Ø9)XLE(1),SIGMA(1)
     WRITE(ND,1966)X,XMAX
```

```
      WRITE(ND,1967)PRNT,DXMIN
      LL=ITURB+2
      GO TO (1991,1999,1945,1978,1926,1933,9950,8000),LL
 1991 WRITE(ND,1959)
      GO TO 2999
 1999 WRITE(ND,1960)XK2
      GO TO 2999
 1945 WRITE(ND,1961)XK2
      GO TO 2999
 1978 WRITE(ND,1962)XK2
      GO TO 2999
 1926 GO TO 2999
 1933 GO TO 2999
 8000 WRITE(ND,8001)
 8001 FORMAT(1H0,22X,30HDONALDSON/GRAY VISCOSITY MODEL)
      GO TO 2999
 9950 WRITE(ND,9951)XK2
 2999 CONTINUE
      WRITE(ND,1916)
      WRITE(ND,1906)T(1),T(MPSI)
      WRITE(ND,1907)U(1),U(MPSI)
      WTMIX(1)=0.0
      WTMIX(MPSI)=0.0
      DO 1930 J=1,NS
      WTMIX(1)=WTMIX(1)+ALPHA(J,1)
 1930 WTMIX(MPSI)=WTMIX(MPSI)+ALPHA(J,MPSI)
      DO 1919 J=1,NS
      RALPHA(J,1)=ALPHA(J,1)/WTMIX(1)
      RALPHA(J,MPSI)=ALPHA(J,MPSI)/WTMIX(MPSI)
 1919 WRITE(ND,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)
      WRITE(ND,120)
      DO 159 I=1,NR
      L=IRR(I)
      GO TO(131,132,133,134,135,136,137,138,139,140),L
  131 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      WRITE(ND,121)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)
      GO TO 159
  132 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,122)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
  133 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
      WRITE(ND,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=
     11,3)
      GO TO 159
  134 J1=IRRR(I,1)
      J2=IRRR(I,2)
```

```
      J3=IRRR(I,3)
      WRITE(ND,124)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
  135 J1=IRRR(I,1)
      J2=IRRR(I,3)
      J3=IRRR(I,4)
      WRITE(ND,125)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
  136 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      WRITE(ND,126)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)
      GO TO 159
  137 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,127)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
  138 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
      WRITE(ND,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=
     11,3)
      GO TO 159
  139 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,129)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
  14Ø J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,13Ø)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
  159 CONTINUE
  12Ø FORMAT(1HØ,19X,26HREACTIONS BEING CONSIDERED,6X,19HKR=A*EXP(B/RT)/
     1T**N,7X,1HA,8X,1HN,9X,1HB,7X,23H(MOLECULE-ML-SEC UNITS))
  121 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1E1Ø.4,2X
     1,F4.1,2X,F1Ø.1)
  122 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,
     1E1Ø.4,2X,F4.1,2X,F1Ø.1)
  123 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,1ØX,
     1E9.3,2X,F4.1,2X,F1Ø.1)
  124 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,E9.3,2X,F4.1,2X,F1Ø.1)
  125 FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,
     1E9.3,2X,F4.1,2X,F1Ø.1)
  126 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,E9.3,2X,
     1F4.1,2X,F1Ø.1,3X,16HONE WAY REACTION)
  127 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H& M,23X,
     1E9.3,2X,F4.1,2X,F1Ø.1,3X,16HONE WAY REACTION)
  128 FORMAT( I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,1ØX,
     1 E9.3,2X,F4.1,2X,F1Ø.1,3X,16HONE WAY REACTION)
  129 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,E9.3,2X,F4.1,2X,F1Ø.1,3
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     1X,16HONE WAY REACTION)
 13Ø FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,E9.3,
     12X,F4.1,2X,F1Ø.1,3X,16HONE WAY REACTION)
19Ø1 FORMAT(1H1,37X,46HAEROCHEM RESEARCH LABORATORIES  PRINCETON N.J.)
19Ø2 FORMAT(35X,5ØHAXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY)
19Ø3 FORMAT(1HØ,24X,1ØA8)
19Ø4 FORMAT(1HØ,22X,19HPRESSURE(INITIAL) =  E15.7,12H ATMOSPHERES)
19Ø5 FORMAT(1HØ,22X,2ØHPRESSURE(CONSTANT) =  E15.7,12H ATMOSPHERES)
19Ø6 FORMAT(23X,24HTEMPERATURE(DEG. KELVIN),3X,  E15.7,4X,  E15.7)
19Ø7 FORMAT(23X,24HVELOCITY (METERS/SECOND),3X,  E15.7,4X,  E15.7)
19Ø8 FORMAT(1HØ,22X,14HNOZZLE RADIUS=  E15.7,7H METERS)
19Ø9 FORMAT(1HØ,22X,23HLEWIS NUMBER(CONSTANT)=  E15.7,5X,25HPRANDTL NUM
    1BER(CONSTANT)=  E15.7)
1916 FORMAT(1HØ,54X,3HJET,16X,4HEDGE)
1917 FORMAT(23X,13HMOLE FRACTION,3X,A6,5X,  E15.7,4X,  E15.7)
1959 FORMAT(1HØ,22X,4ØHLAMINAR VISCOSITY MODEL(SUTHERLANDS LAW))
196Ø FORMAT(1HØ,22X,29HCONSTANT VISCOSITY MODEL  MU=  E15.7)
1962 FORMAT(1HØ,22X,31HTING-LIBBY VISCOSITY MODEL    K=  E15.7)
1961 FORMAT(1HØ,22X,27HFERRI VISCOSITY MODEL       K=  E15.7)
1966 FORMAT(/,22X,18HX INITIAL(METERS)=,E15.7,12X,16HX FINAL(METERS)=,
    *E15.7)
1967 FORMAT(1HØ,22X,16HPRINT INCREMENT=  E15.7,12X,18HMINIMUM STEP SIZE
    1=  E15.7)
9951 FORMAT(1HØ,22X,69HTING-LIBBY VISCOSITY MODEL AFTER MIXING REGION I
    1NTERSECTS X AXIS    K=  E15.7)
     X=X/AMULT
     XMAX=XMAX/AMULT
     PRNT=PRNT/AMULT
     RJ=RJ/AMULT
     DXMIN=DXMIN/AMULT
     DO 7667 I=1,MPSI
7667 U(I)=U(I)/AMULT
     RETURN
     END
     SUBROUTINE GRATE(ANSWER,Y,X,N)
     DIMENSION X(3Ø),Y(5Ø)
     COMMON/UNITS/NNDUM(15),ND
     SUM = Ø.Ø
     INTER = N-1
     I1 = 1
     I2 = 2
     DO 1 I = 1,INTER
     SUM = SUM + (X(I2)-X(I1))*(Y(I2)+Y(I1))
     I1 = I1 + 1
     I2 = I2 + 1
   1 CONTINUE
     ANSWER = Ø.5*SUM
     RETURN
     END
     SUBROUTINE  TICK(JJJJ)
     CALL SECOND(TIME)
     JJJJ=TIME
     RETURN
     END
     SUBROUTINE SLDP(X,A,N)
```

```
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR
C     EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE
C     DIAGONAL PIVOT STRATEGY
      DIMENSION A(25,25),X(25)
      COMMON/UNITS/ NNDUM(14),ND,NDBG
      DO 9 K=1,N
      IF (ABS(A(K,K)) .GT. 1.E-1Ø) GO TO 5
      WRITE(NDBG,1Ø1)
      GO TO 99
    5 KP1= K+1
      DO 6 J= KP1, N
    6 A(K,J)= A(K,J)/A(K,K)
      X(K)= X(K)/A(K,K)
      A(K,K)= 1.Ø
      DO 9 I=1,N
      IF (I.EQ.K .OR. A(I,K).EQ.Ø.) GO TO 9
      DO 8 J=KP1,N
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)
      X(I)= X(I)- A(I,K)*X(K)
      A(I,K)=Ø.
    9 CONTINUE
   99 CONTINUE
  1Ø1 FORMAT( 22H ERROR--- SMALL PIVOT )
      RETURN
      END
      SUBROUTINE TKEY(T,TTB,ITKEY,SDT,HDT,NT,J)
      DIMENSION TTB(3Ø,24)
      COMMON/UNITS/NNDUM(15),NDBG
      NT1=NT-1
      DO 1Ø IT=1,NT1
      DT= TTB(IT+1,J)-TTB(IT,J)
      SDT=(T-TTB(IT,J))/DT
      HDT=(TTB(  IT+1,J)-T) /DT
      IF ((SDT*HDT).GE.Ø.Ø) GO TO 11
   1Ø CONTINUE
      WRITE(NDBG,1ØØ) T,IT
      ITKEY=Ø
  1ØØ FORMAT(1H , 28H   TEMPERATURE OUT OF RANGE , E14.5,I5)
      RETURN
   11 ITKEY=IT
      RETURN
      END
      SUBROUTINE LIPLN(ITKEY,I,ATB,SDT,HDT,AX)
      DIMENSION ATB(25,3Ø)
      AX= ATB(I,ITKEY)*HDT+ ATB(I,ITKEY+1)*SDT
      RETURN
      END
```

APPENDIX K

MEFF, BLAKE, LAPP OUTPUT LISTING

```
155-MM HOWITZER WITH M203 CHARGE

MUZZLE VELOCITY VO = 807.7     M/SEC
BORE LENGTH L = 5.080     METERS
PROPELLANT MASS MP = 12.23     KG
PROJECTILE MASS W = 46.36     KG
GUN CALIBER  CALBER = 156.5     MM
BARREL CROSS SECTIONAL AREA A = .1924E-01 M**2
SPECIFIC HEAT RATIO OF PROPELLANT GAS  GAM = 1.241
MEAN MOLECULAR WEIGHT OF PROPELLANT GAS  MBAR = 23.43
AVERAGE BARREL GAS TEMPERATURE  TA = 1860.     DEG K
COVOLUME ETA = .1041E-02 M**3/KG
CHAMBER VOLUME CVO = .1966E-01 M**3


          MUZZLE GAS PROPERTIES WHEN PROJECTILE IS EJECTED


               PRESSURE=   694.21 ATM
               TEMPERATURE=   1828.2 K
               VELOCITY=    807.7 M/SEC


          MUZZLE GAS PROPERTIES WHEN MUZZLE VELOCITY BECOMES SONIC


               PRESSURE=   554.38 ATM
               TEMPERATURE=   1749.0 K
               VELOCITY=    877.7 M/SEC
               FRACTION OF EJECTED PROPELLANT=   .0095


          FLOW CONDITIONS AT REFLECTED SHOCK WHEN MUZZLE VELOCITY BECOMES SONIC

               PRESSURE=     1.00 ATM
               TEMPERATURE=    512.8 K
               VELOCITY=   2299.8 M/SEC
               FRACTION OF GAS ENTERING REFLECTED SHOCK=   .8159

          FLOW CONDITIONS AT NORMAL SHOCK WHEN MUZZLE VELOCITY BECOMES SONIC
```

```
PRESSURE=     1.00 ATM
TEMPERATURE=   1934.1 K
VELOCITY=    306.0 M/SEC
```

FLOW CONDITIONS AT MIXING REGION BOUNDARY WHEN MUZZLE VELOCITY BECOMES SONIC

```
PRESSURE=     1.00 ATM
TEMPERATURE=    987.9 K
VELOCITY=   1932.8 M/SEC
BOUNDARY RADIUS =    .933 M
```

MACH NO IS .GE. 1

```
**  PROGRAM BLAKE, VERSION  205.11  **

TIGER! TIGER! BURNING BRIGHT/ IN THE FORESTS OF THE NIGHT,
WHAT IMMORTAL HAND OR EYE/ DARE FRAME THY FEARFUL SYMMETRY?
                     ---WILLIAM BLAKE (1757-1827)

                 25 AUG, 1983

**NOTE:  THE USE OF ENGLISH UNITS IS TO BE DEPRECATED. SI UNITS ARE COMING.  YOU WON'T LEARN THEM IF YOU DON'T USE THEM  !

* *       USING THE BINARY LIBRARY CREATED ON  12 NOV, 1982       * *
```

M30A1

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1260	27.900	.018	-1.6916E+08	C 6000 H 7549 O 9901 N 2451
NG	22.420	17.201	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	46.840	78.418	-2.2100E+04	C 1 H 4 O 2 N 4
EC	1.490	.967	-2.5100E+04	C 17 H 20 O 1 N 2
KS	1.000	1.000	-3.4266E+05	K 2 S 1 O 4
ALC	.250	.945	-6.6420E+04	C 2 H 6 O 1
C	.100	1.451	0.	C 1

THE HEAT OF FORMATION IS -384.86 CAL/GRAM = -6.7053E+04 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	14.896
H	32.439
O	28.660
N	23.830
K	.116
S	.058

M30A1

THERE ARE 29 GASEOUS CONSTITUENTS SELECTED

	NAME	BKW CO-VOL	L-J EPS/K	L-J SIGMA	A1	A2	A3	A4	A5	A6	A7	A8	A9
							THERMO CONSTANTS						
1.	CO	390.0	91.7	3.690	5.83775	-.40270	.06491	-.00373	-2.14066	.71717	-.08241	-31130.5	53.1746
2.	H2O	250.0	542.5	2.790	7.60069	.39388	-.10260	.00807	-4.86836	2.30899	-.37689	-62860.1	47.1008
3.	CO2	600.0	195.2	3.941	9.06744	-.40694	.06138	-.00273	-2.70529	.56199	-.04428	-102647.7	60.2574
4.	N2	380.0	71.4	3.798	5.90618	-.39603	.05863	-.00307	-2.41322	.69566	-.11540	-4569.1	51.2456
5.	H2	180.0	59.7	2.827	4.48064	.19824	-.00851	-.00003	-1.97442	1.15151	-.21216	-2116.7	36.2744
6.	NO	386.0	116.7	3.492	5.77838	-.43892	.08202	-.00561	-1.79245	.50895	-.04564	16765.3	57.0969
7.	KOH	0.0	100.0	3.500	7.27052	.40176	-.10705	.00896	-1.70167	.87842	-.16291	-59999.7	68.1294
8.	NH3	476.0	558.3	2.900	13.60829	-.93312	.18185	-.00958	-9.06058	3.51672	-.50840	-22985.7	45.5074
9.	HCN	359.0	344.7	3.339	9.48792	-.37343	.04424	-.00222	-4.59416	1.73907	-.25679	24383.5	53.6459
10.	CH4	528.0	148.6	3.758	20.35251	-1.95871	.26284	-.01397	-14.43248	5.11197	-.67906	-38010.8	38.5449
11.	COS	0.0	100.0	3.500	9.07572	-.47894	.09730	-.00658	-2.27231	.48548	-.04719	-41172.7	66.5255
12.	C2H4	372.0	224.7	4.163	22.63477	-1.64131	.20002	-.00937	-13.78191	4.49325	-.59268	-10548.7	51.3360
13.	C2H2	0.0	100.0	3.500	12.54985	-.16675	.02155	-.00023	-5.90900	2.01409	-.26643	43014.0	54.7220
14.	O2	350.0	106.7	3.467	2.20306	1.12042	-.18485	.01276	2.02364	-1.20737	.22334	-2085.5	59.2300
15.	K	0.0	100.0	3.500	6.09867	-1.44727	.10388	.03850	-3.46738	1.37555	-.18637	16559.0	41.4178
16.	S	0.0	100.0	3.500	1.83331	.19365	.01065	-.00358	.77619	-.26477	.03824	65713.8	47.5476
17.	C2N2	0.0	100.0	3.500	13.82927	-1.13108	.19089	-.01258	-5.06809	1.56648	-.19796	61813.4	70.4037
18.	OH	226.0	100.0	3.500	4.22400	.47240	-.11211	.00942	-1.70189	.97134	-.16944	7437.0	49.0478
19.	KO	0.0	100.0	3.500	4.49837	.11393	.00019	-.00002	.00503	-.02588	.00186	14185.2	67.4039
20.	SO	0.0	100.0	3.500	1.92172	1.33802	-.22714	.01363	2.24044	-1.13902	.18518	-219.7	63.6970
21.	S2	0.0	100.0	3.500	4.48800	.03544	-.00050	.00003	.02430	-.11854	.01769	27643.9	64.5607
22.	HS	0.0	100.0	3.500	6.12907	-.41325	.06726	-.00371	-2.95581	1.32672	-.19604	30547.3	51.9361
23.	CH3	525.0	100.0	3.500	13.82287	-.74765	.05695	-.00032	-9.14376	3.65133	-.54025	23004.1	46.4265
24.	H	13.4	100.0	3.500	2.49993	.00000	-.00000	.00000	.00000	-.00000	.00000	50621.8	33.4041
25.	O	212.8	100.0	3.500	2.97972	-.25641	.05953	-.00389	-.43119	.19753	-.02943	57760.7	44.3789
26.	CHO	700.0	100.0	3.500	10.04357	-1.09647	.20969	-.01480	-4.57561	1.36019	-.14753	955.9	59.4686
27.	CH2	525.0	100.0	3.500	11.42150	-1.32276	.21610	-.01403	-7.38097	3.01187	-.44496	83047.1	47.9048
28.	CN	0.0	100.0	3.500	2.71179	.54169	.09568	-.02040	1.50282	-1.01851	.20537	101465.0	58.3631
29.	K2	0.0	100.0	3.500	4.50198	.24737	.00004	.00000	-.00245	-.00020	-.00023	27675.0	70.3214

THE FLOOR IS AT 14

M30A1

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

	P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHO (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP
1)	.100000E+01	6781.3218	1934.	-598.50	-762.72	2.693	.000	.357	4.187	4.181	1.240

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		1)
N2	GAS	1.17932E+01
CO	GAS	1.08207E+01
H2O	GAS	9.63504E+00
H2	GAS	6.37568E+00
CO2	GAS	3.91796E+00
KOH	GAS	5.35738E-02
COS	GAS	4.81146E-03
NO	GAS	1.00016E-04
NH3	GAS	2.97012E-05
O2	GAS	3.17973E-06
HCN	GAS	2.44635E-06
CH4	GAS	1.15941E-08
C2H4	GAS	0.
C2H2	GAS	0.
K	GAS	6.11977E-02
S	GAS	1.46775E-03
C2N2	GAS	0.
OH	GAS	2.21924E-03
KO	GAS	2.64480E-06
SO	GAS	1.46835E-02
S2	GAS	1.19222E-02
HS	GAS	1.25803E-02
CH3	GAS	0.
H	GAS	1.71882E-02
O	GAS	4.45821E-06
CHO	GAS	1.75940E-06
CH2	GAS	0.
CN	GAS	0.
K2	GAS	2.91199E-07

TOTAL GAS (MOLES/KG) 42.7226

M3CA1

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

	P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHO (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP
1)	.694204E+03	10.2418	1828.	-634.45	-806.63	2.111	.098	.347	3.987	3.573	1.396

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		1)
N2	GAS	1.17775E+01
CO	GAS	1.06925E+01
H2O	GAS	9.54839E+00
H2	GAS	6.37242E+00
CO2	GAS	3.98099E+00
KOH	GAS	1.10894E-01
COS	GAS	5.27317E-02
NO	GAS	1.00175E-06
NH3	GAS	2.94718E-02
O2	GAS	0.
HCN	GAS	2.15448E-03
CH4	GAS	1.51000E-02
C2H4	GAS	3.37669E-06
C2H2	GAS	1.90387E-06
K	GAS	3.87803E-03
S	GAS	6.84639E-06
C2N2	GAS	3.95391E-09
OH	GAS	2.56511E-05
KO	GAS	6.79464E-08
SO	GAS	7.06865E-05
S2	GAS	9.75216E-04
HS	GAS	2.62794E-03
CH3	GAS	1.58578E-05
H	GAS	2.64819E-04
O	GAS	0.
CHO	GAS	2.79025E-05
CH2	GAS	0.
CN	GAS	2.01530E-09
K2	GAS	1.11125E-06

TOTAL GAS (MOLES/KG) 42.5905

ALPHA=	.816
H2O	2.245E-01
CO	2.515E-01
H2	1.496E-01
N2	2.765E-01
CO2	9.318E-02
H	7.920E-05
OH	1.006E-05
O	1.923E-08
O2	1.371E-08
K	3.382E-04
KOH	2.356E-03
KO2	0.
HO2	0.

```
                    AERUCHEM RESEARCH LABORATORIES  PRINCETON N.J.
                 AXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY

      155-MM HOWITZER WITH M203 CHARGE

    PRESSURE(CONSTANT) =    .1000000F+01 ATMOSPHERES

    NOZZLE RADIUS=   .9330000E+00 METERS

    LEWIS NUMBER(CONSTANT)=   .1000000E+01      PRANDTL NUMBER(CONSTANT)=   .1000000F+01

   X INITIAL(METERS)=  0.                        X FINAL(METERS)=   .5000000E+02

    PRINT INCREMENT=   .5000000E+01             MINIMUM STEP SIZE=   .1000000E-10

    DONALDSON/GRAY VISCOSITY MODEL

                                          JET               EDGE
    TEMPERATURE(DEG. KELVIN)        .9878710E+03       .2940000E+03
    VELOCITY (METERS/SECOND)        .1932812E+04       .3000000E+01
    MOLE FRACTION   H2O             .2249356E+00       .9996801E-51
    MOLE FRACTION   CO              .2519880E+00       .9996801E-51
    MOLE FRACTION   H2              .1498903E+00       .9996801E-51
    MOLE FRACTION   N2              .2770365E+00       .7897473E+00
    MOLE FRACTION   CO2             .9336079E-01       .3198976E-03
    MOLE FRACTION   H               .7935367E-04       .9996801E-51
    MOLE FRACTION   OH              .1007952E-04       .9996801E-51
    MOLE FRACTION   O               .1926731E-07       .9996801E-51
    MOLE FRACTION   O2              .1373660E-07       .2099328E+00
    MOLE FRACTION   K               .3388562E-03       .9996801E-51
    MOLE FRACTION   KOH             .2360571E-02       .9996801E-51
    MOLE FRACTION   KO2             .1001940E-98       .9996801E-51
    MOLE FRACTION   HO2             .1001940E-98       .9996801E-51

   REACTIONS BEING CONSIDERED      KR=A*EXP(B/RT)/T**N          A         N         B      (MOLECULE-ML-SEC UNITS)
 1   CO   + O    + M  = CO2  + M                          .7000E-32   0.0    -4369.0
 2   CO   + O2        = CO2  + O                          .4200E-11   0.0   -47664.0
 3   O    + O    + M  = O2   + M                          .3000E-33   0.0     1792.0
 4   CO   + OH        = CO2  + H                          .2800E-16  -1.3      660.0
 5   OH   + H2        = H2O  + H                          .1900E-14  -1.3    -3626.0
 6   H    + O2        = OH   + O                          .2400E-09   0.0   -16393.0
 7   O    + H2        = OH   + H                          .3000E-13  -1.0    -8902.0
 8   OH   + OH        = H2O  + O                          .1050E-10   0.0    -1093.0
 9   H    + H    + M  = H2   + M                          .3000E-29   1.0        0.0
10   H    + OH   + M  = H2O  + M                          .1000E-24   2.0        0.0
11   H    + O2   + M  = HO2  + M                          .1500E-31   0.0      994.0
12   H    + HO2       = OH   + OH                         .1700E-09   0.0     -994.0
13   CO   + HO2       = CO2  + OH                         .2500E-09   0.0   -23645.0
14   H    + HO2       = H2   + O2                         .4200E-10   0.0     -695.0
15   H    + HO2       = H2O  + O                          .8500E-11   0.0     -994.0
16   OH   + HO2       = H2O  + O2                         .3000E-10   0.0        0.0
17   O    + HO2       = OH   + O2                         .3500E-10   0.0        0.0
18   O    + H    + M  = OH   + M                          .1000E-28   1.0        0.0
19   HO2  + H2        = H2O  + OH                         .1000E-11   0.0   -18678.0
20   H    + KOH       = H2O  + K                          .1800E-10   0.0    -1987.0
21   K    + OH   + M  = KOH  + M                          .1500E-26   1.0        0.0
22   KO2  + OH        = KOH  + O2                         .2000E-10   0.0        0.0
23   K    + O2   + M  = KO2  + M                          .3000E-29   1.0        0.0
24   K    + HO2       = KO2  + H                          .1000E-10   0.0   -13000.0
25   KO2  + H2        = KOH  + OH                         .3000E-11   0.0   -19870.0
```

X= 0. METERS 155-MM HOWITZER WITH M203 CHARGE

X/R	DELTA X METERS	PRESS(ATM)
0.	.933000E-01	.100000E+01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
.227167E+01	.112717E+01	.184557E+01	.248000E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	0.	1
2	.1000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.220549E+01	2
3	.2000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.441098E+01	3
4	.3000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.661647E+01	4
5	.4000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.882196E+01	5
6	.5000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.110275E+02	6
7	.6000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.132329E+02	7
8	.7000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.154384E+02	8
9	.8000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.176439E+02	9
10	.9000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.198494E+02	10
11	1.0000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.220549E+02	11
12	3.5433	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.305634E+02	.242604E+02	12
13	7.6940	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.305634E+02	.264659E+02	13

X = 0. METERS 155-MM HOWITZER WITH M203 CHARGE PAGE 1

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	1
2	.10000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	2
3	.20000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	3
4	.30000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	4
5	.40000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	5
6	.50000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	6
7	.60000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	7
8	.70000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	8
9	.80000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	9
10	.90000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	10
11	1.00000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	11
12	3.54334	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	12
13	7.69399	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	13

X= 0. METERS 155-MM HOWITZER WITH M203 CHARGE

MOLE FRACTIONS

PT	Y/R	O	O2	K	KOH	KO2	HO2		PT
1	0.00000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	1
2	.10000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	2
3	.20000	.19267E-07	.13737E-07	.33686E-03	.23606E-02	.10019E-98	.10019E-98	0.	3
4	.30000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	4
5	.40000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	5
6	.50000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	6
7	.60000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	7
8	.70000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	8
9	.80000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	9
10	.90000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	10
11	1.00000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	0.	11
12	3.54334	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	0.	12
13	7.69399	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	0.	13

X/R	DELTA X METERS	PRESS(ATM)
.107355E+02	.206823E-01	.100000E+01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
.115144E+01	.540351E+00	.147341E+01	.248000E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.192714E+04	.990368E+03	.288604E+00	.285557E+01	-.978827E+03	.392487E+01	0.	1
2	.1003	.192570E+04	.990773E+03	.288530E+00	.285310E+01	-.977848E+03	.392387E+01	.220549E+01	2
3	.2007	.192075E+04	.992158E+03	.288278E+00	.284458E+01	-.974473E+03	.392044E+01	.441098E+01	3
4	.3016	.190998E+04	.995126E+03	.287741E+00	.282612E+01	-.967126E+03	.391313E+01	.661647E+01	4
5	.4032	.188914E+04	.100074E+04	.286740E+00	.279063E+01	-.952884E+03	.389953E+01	.882196E+01	5
6	.5066	.185142E+04	.101048E+04	.285064E+00	.272713E+01	-.927051E+03	.387673E+01	.110275E+02	6
7	.6128	.178696E+04	.102590E+04	.282613E+00	.262103E+01	-.883311E+03	.384340E+01	.132329E+02	7
8	.7241	.168248E+04	.104729E+04	.279783E+00	.245539E+01	-.813876E+03	.380491E+01	.154384E+02	8
9	.8437	.152236E+04	.107036E+04	.278286E+00	.221503E+01	-.711406E+03	.378456E+01	.176439E+02	9
10	.9762	.129417E+04	.107922E+04	.282661E+00	.189545E+01	-.574240E+03	.384405E+01	.198494E+02	10
11	1.1273	.100623E+04	.103625E+04	.303443E+00	.152206E+01	-.416596E+03	.412667E+01	.220549E+02	11
12	1.3025	.707100E+03	.918336E+03	.353492E+00	.114750E+01	-.271100E+03	.480732E+01	.242604E+02	12
13	1.5071	.457755E+03	.760228E+03	.438940E+00	.821422E+00	-.164616E+03	.596937E+01	.264659E+02	13
14	1.7488	.281450E+03	.608745E+03	.559271E+00	.565663E+00	-.972430E+02	.760580E+01	.286714E+02	14
15	2.0419	.166621E+03	.489951E+03	.704186E+00	.373766E+00	-.562974E+02	.957658E+01	.308769E+02	15
16	2.4167	.935390E+02	.405924E+03	.857268E+00	.230896E+00	-.318055E+02	.116584E+02	.330824E+02	16
17	2.9406	.477679E+02	.349976E+03	.999726E+00	.127043E+00	-.166480E+02	.135958E+02	.352879E+02	17
18	3.7817	.205787E+02	.316007E+03	.111078E+01	.576562E-01	-.775438E+01	.151060E+02	.374933E+02	18
19	5.3126	.790298E+01	.300098E+03	.117143E+01	.227326E-01	-.360440E+01	.159309E+02	.396988E+02	19
20	7.7739	.413328E+01	.295394E+03	.119062E+01	.119853E-01	-.236115E+01	.161919E+02	.419043E+02	20
21	10.5817	.328819E+01	.294350E+03	.119497E+01	.955199E-02	-.207973E+01	.162509E+02	.441098E+02	21
22	13.1111	.308263E+01	.294100E+03	.119601E+01	.895875E-02	-.201057E+01	.162652E+02	.463153E+02	22
23	15.4433	.302242E+01	.294027E+03	.119632E+01	.878486E-02	-.199012E+01	.162694E+02	.485208E+02	23
24	17.5407	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.162709E+02	.507263E+02	24

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.22454E+00	.25140E+00	.14951E+00	.27828E+00	.93153E-01	.70257E-07	.24896E-08	1
2	.10029	.22441E+00	.25125E+00	.14941E+00	.27859E+00	.93099E-01	.81986E-07	.29694E-08	2
3	.20070	.22397E+00	.25072E+00	.14909E+00	.27968E+00	.92913E-01	.11865E-06	.45107E-08	3
4	.30155	.22300E+00	.24959E+00	.14838E+00	.28203E+00	.92505E-01	.18415E-06	.74196E-08	4
5	.40324	.22110E+00	.24737E+00	.14701E+00	.28658E+00	.91711E-01	.28220E-06	.12122E-07	5
6	.50658	.21762E+00	.24332E+00	.14452E+00	.29486E+00	.90260E-01	.42066E-06	.19326E-07	6
7	.61284	.21158E+00	.23631E+00	.14021E+00	.30914E+00	.87750E-01	.63522E-06	.31297E-07	7
8	.72415	.20162E+00	.22472E+00	.13312E+00	.33266E+00	.83615E-01	.10764E-05	.57851E-07	8
9	.84370	.18596E+00	.20647E+00	.12191E+00	.36968E+00	.77114E-01	.24085E-05	.15113E-06	9
10	.97616	.16271E+00	.17940E+00	.10529E+00	.42461E+00	.67447E-01	.70341E-05	.61467E-06	10
11	1.12733	.13059E+00	.14356E+00	.84039E-01	.49751E+00	.54211E-01	.39724E-05	.56197E-06	11
12	1.30255	.94183E-01	.10415E+00	.61300E-01	.57779E+00	.39237E-01	.16043E-06	.43830E-07	12
13	1.50708	.62337E-01	.69215E-01	.40880E-01	.64892E+00	.26086E-01	.23163E-08	.20354E-08	13
14	1.74883	.38872E-01	.43267E-01	.25606E-01	.70173E+00	.16389E-01	.12474E-10	.49052E-10	14
15	2.04187	.23122E-01	.25775E-01	.15273E-01	.73732E+00	.98784E-02	.36111E-13	.64481E-12	15
16	2.41673	.12909E-01	.14405E-01	.85428E-02	.76045E+00	.56566E-02	.95285E-16	.66033E-14	16
17	2.94058	.64075E-02	.71549E-02	.42455E-02	.77520E+00	.29688E-02	.36170E-18	.86119E-16	17
18	3.78168	.25232E-02	.28190E-02	.16734E-02	.78401E+00	.13630E-02	.23691E-20	.20075E-17	18
19	5.31257	.70463E-03	.78752E-03	.46763E-03	.78815E+00	.61120E-03	.26463E-22	.94573E-19	19
20	7.77393	.16290E-03	.18213E-03	.10818E-03	.78938E+00	.38725E-03	.24551E-23	.39789E-19	20
21	10.58171	.41423E-04	.46322E-04	.27519E-04	.78965E+00	.33702E-03	.13395E-23	.86313E-19	21
22	13.11106	.11876E-04	.13283E-04	.78920E-05	.78972E+00	.32481E-03	.31483E-24	.70957E-19	22
23	15.44331	.32214E-05	.36033E-05	.21411E-05	.78974E+00	.32123E-03	.36408E-25	.30280E-19	23
24	17.54072	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	24

MOLE FRACTIONS

PT	Y/R	O	O2	K	KOH	KO2	HO2		PT
1	0.00000	.34911E-10	.43172E-03	.37470E-03	.22662E-02	.52256E-04	.10977E-06	0.	1
2	.10029	.51761E-10	.54617E-03	.36513E-03	.22648E-02	.61653E-04	.15389E-06	0.	2
3	.20070	.13081E-09	.94454E-03	.33567E-03	.22598E-02	.90595E-04	.32192E-06	0.	3
4	.30155	.39885E-09	.18270E-02	.28555E-03	.22485E-02	.13992E-03	.73271E-06	0.	4
5	.40324	.12256E-08	.35752E-02	.21945E-03	.22255E-02	.20544E-03	.15684E-05	0.	5
6	.50658	.36231E-08	.68134E-02	.15114E-03	.21810E-02	.27519E-03	.30343E-05	0.	6
7	.61284	.10689E-07	.12472E-01	.98595E-04	.20984E-02	.33588E-03	.54796E-05	0.	7
8	.72415	.35106E-07	.21850E-01	.72611E-04	.19506E-02	.38663E-03	.10193E-04	0.	8
9	.84370	.15111E-06	.36621E-01	.73143E-04	.17003E-02	.44276E-03	.21999E-04	0.	9
10	.97616	.81789E-06	.58556E-01	.90222E-04	.13353E-02	.50329E-03	.52117E-04	0.	10
11	1.12733	.77167E-06	.88474E-01	.30925E-04	.10678E-02	.44604E-03	.73217E-04	0.	11
12	1.30255	.42813E-07	.12218E+00	.11203E-05	.84148E-03	.27670E-03	.45865E-04	0.	12
13	1.50708	.83956E-09	.15179E+00	.98037E-08	.58292E-03	.16019E-03	.23757E-04	0.	13
14	1.74883	.18056E-10	.17366E+00	.23216E-10	.37282E-03	.91413E-04	.11746E-04	0.	14
15	2.04187	.58936E-12	.18835E+00	.20122E-13	.22518E-03	.51263E-04	.57105E-05	0.	15
16	2.41673	.22873E-13	.19788E+00	.15164E-16	.12696E-03	.27494E-04	.26767E-05	0.	16
17	2.94058	.92065E-15	.20395E+00	.24435E-19	.63437E-04	.13266E-04	.11388E-05	0.	17
18	3.78168	.36116E-16	.20758E+00	.67072E-22	.25099E-04	.51169E-05	.39015E-06	0.	18
19	5.31257	.17315E-17	.20927E+00	.22124E-24	.70339E-05	.14066E-05	.95690E-07	0.	19
20	7.77393	.15576E-17	.20978E+00	.48725E-26	.16306E-05	.32117E-06	.19513E-07	0.	20
21	10.58171	.45314E-17	.20989E+00	.67919E-27	.41549E-06	.80902E-07	.44301E-08	0.	21
22	13.11106	.41305E-17	.20992E+00	.49374E-28	.11928E-06	.23049E-07	.11633E-08	0.	22
23	15.44331	.18697E-17	.20993E+00	.27455E-29	.32381E-07	.62301E-08	.29899E-09	0.	23
24	17.54072	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	0.	24

X= .1528463E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

X/R	DELTA X METERS	PRESS(ATM)
.163822E+02	.559850E-01	.100000E+01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
.136568E+01	.423064E+00	.108226E+01	.253723E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.184212E+04	.102239E+04	.282216E+00	.270083E+01	-.920967E+03	.578919E+01	0.	1
2	.2100	.182014E+04	.103968E+04	.278395E+00	.265172E+01	-.906808E+03	.571081E+01	.441098E+01	2
3	.4279	.174858E+04	.112531E+04	.260475E+00	.247059E+01	-.863678E+03	.534322E+01	.882196E+01	3
4	.6805	.160169E+04	.139032E+04	.218487E+00	.208955E+01	-.790092E+03	.448191E+01	.132329E+02	4
5	.9949	.133226E+04	.165183E+04	.194340E+00	.164917E+01	-.668194E+03	.398656E+01	.176439E+02	5
6	1.4211	.861339E+03	.205680E+04	.170414E+00	.100413E+01	-.415905E+03	.349576E+01	.220549E+02	6
7	1.9766	.477823E+03	.121281E+04	.285225E+00	.704572E+00	-.216745E+03	.585092E+01	.264659E+02	7
8	2.4337	.267291E+03	.677657E+03	.506121E+00	.512861E+00	-.955539E+02	.103823E+02	.308769E+02	8
9	2.9690	.143056E+03	.485161E+03	.713953E+00	.323042E+00	-.479955E+02	.146456E+02	.352879E+02	9
10	3.6754	.683061E+02	.381366E+03	.915418E+00	.173935E+00	-.228944E+02	.187783E+02	.396988E+02	10
11	4.8835	.260869E+02	.324552E+03	.108086E+01	.721078E-01	-.929929E+01	.221721E+02	.441098E+02	11
12	7.3260	.831827E+01	.300970E+03	.116799E+01	.238923E-01	-.367103E+01	.239593E+02	.485208E+02	12
13	11.5966	.396635E+01	.295254E+03	.119121E+01	.115041E-01	-.229116E+01	.244358E+02	.529318E+02	13
14	16.5122	.319675E+01	.294253E+03	.119537E+01	.928795E-02	-.204571E+01	.245211E+02	.573428E+02	14
15	20.7953	.304371E+01	.294056E+03	.119620E+01	.884631E-02	-.199657E+01	.245380E+02	.617537E+02	15
16	24.7941	.300588E+01	.294008E+03	.119640E+01	.873709E-02	-.198435E+01	.245422E+02	.661647E+02	16
17	28.3697	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.245428E+02	.705757E+02	17

X = .1528463E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.21805E+00	.24200E+00	.14294E+00	.29713E+00	.90463E-01	.71503E-06	.32498E-07	1
2	.21004	.21764E+00	.23898E+00	.14029E+00	.30227E+00	.90538E-01	.13845E-05	.53269E-07	2
3	.42789	.21950E+00	.22674E+00	.12924E+00	.31997E+00	.93837E-01	.32376E-04	.80314E-06	3
4	.68049	.22673E+00	.18722E+00	.10394E+00	.36108E+00	.11707E+00	.11205E-02	.43026E-04	4
5	.99490	.22694E+00	.12832E+00	.63712E-01	.43874E+00	.13910E+00	.46524E-03	.73167E-04	5
6	1.42109	.19958E+00	.14888E-01	.30828E-02	.58813E+00	.17377E+00	.50816E-03	.35869E-02	6
7	1.97658	.11017E+00	.38208E-01	.11991E-02	.66812E+00	.64931E-01	.33668E-03	.44997E-03	7
8	2.43368	.42771E-01	.35496E-01	.18879E-01	.71014E+00	.21562E-01	.62703E-07	.15228E-06	8
9	2.96901	.21043E-01	.20961E-01	.11954E-01	.74563E+00	.97240E-02	.13237E-10	.28125E-09	9
10	3.67539	.95688E-02	.10204E-01	.59389E-02	.76875E+00	.43865E-02	.37528E-14	.47145E-12	10
11	4.88349	.33516E-02	.36719E-02	.21571E-02	.78225E+00	.17171E-02	.18447E-17	.11168E-14	11
12	7.32596	.76910E-03	.85153E-03	.50250E-03	.78801E+00	.63853E-03	.14115E-20	.46683E-17	12
13	11.59658	.13945E-03	.15506E-03	.91720E-04	.78943E+00	.37757E-03	.39904E-23	.76359E-19	13
14	16.51219	.28360E-04	.31593E-04	.18711E-04	.78968E+00	.33162E-03	.26048E-24	.24576E-19	14
15	20.79530	.62969E-05	.70210E-05	.41610E-05	.78973E+00	.32250E-03	.26372E-25	.11249E-19	15
16	24.79405	.84699E-06	.94462E-06	.55994E-06	.78975E+00	.32025E-03	.57471E-27	.18534E-20	16
17	28.36967	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	17

MOLE FRACTIONS

PT	Y/R	O	O2	K	KOH	KO2	HO2		PT
1	0.00000	.65801E-08	.68086E-02	.23080E-03	.19991E-02	.36870E-03	.62387E-05	0.	1
2	.21004	.16256E-07	.76922E-02	.42879E-03	.17291E-02	.41767E-03	.10038E-04	0.	2
3	.42789	.50660E-06	.81553E-02	.15391E-02	.55795E-03	.40858E-03	.23864E-04	0.	3
4	.68049	.18781E-05	.41519E-03	.22981E-02	.76232E-04	.37400E-05	.41223E-06	0.	4
5	.99490	.18626E-05	.54475E-03	.17425E-02	.34627E-03	.82884E-06	.23408E-06	0.	5
6	1.42109	.45270E-03	.14518E-01	.42459E-03	.10482E-02	.44536E-06	.21954E-05	0.	6
7	1.97658	.57037E-03	.11516E+00	.26740E-03	.52929E-03	.76444E-05	.54701E-04	0.	7
8	2.43368	.57584E-06	.17064E+00	.22065E-06	.30555E-03	.13812E-03	.68413E-04	0.	8
9	2.96901	.19624E-08	.19042E+00	.52212E-10	.17181E-03	.65752E-04	.22405E-04	0.	9
10	3.67539	.43098E-11	.20104E+00	.17842E-14	.83944E-04	.27702E-04	.68821E-05	0.	10
11	4.88349	.13658E-13	.20681E+00	.95071E-19	.30714E-04	.89459E-05	.16469E-05	0.	11
12	7.32596	.74520E-16	.20922E+00	.15798E-22	.72429E-05	.19121E-05	.27711E-06	0.	12
13	11.59658	.13967E-17	.20980E+00	.79702E-26	.13371E-05	.32729E-06	.39848E-07	0.	13
14	16.51219	.55793E-18	.20991E+00	.11599E-27	.27506E-06	.63848E-07	.68988E-08	0.	14
15	20.79530	.29133E-18	.20993E+00	.52551E-29	.61478E-07	.13817E-07	.13852E-08	0.	15
16	24.79405	.49719E-19	.20993E+00	.40762E-30	.82863E-08	.18434E-08	.18031E-09	0.	16
17	28.36967	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	0.	17

X= .4196607E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

X/R	DELTA X METERS	PRESS(ATM)
.449797E+02	.110148E+00	.100000E+01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
.223268E+01	0.	.663500E+00	.340269E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.102834E+04	.208426E+04	.164578E+00	.117919E+01	-.486691E+03	.597887E+01	0.	1
2	.7658	.945981E+03	.216348E+04	.161016E+00	.107504E+01	-.440738E+03	.584949E+01	.882196E+01	2
3	1.5946	.695635E+03	.201723E+04	.175091E+00	.819497E+00	-.286563E+03	.636079E+01	.176439E+02	3
4	2.5843	.416490E+03	.146771E+04	.240453E+00	.567491E+00	-.161503E+03	.873533E+01	.264659E+02	4
5	3.6764	.239610E+03	.100857E+04	.349043E+00	.387642E+00	-.906074E+02	.126802E+02	.352879E+02	5
6	4.9171	.141692E+03	.720142E+03	.488249E+00	.267612E+00	-.529413E+02	.177374E+02	.441098E+02	6
7	6.3288	.864524E+02	.548144E+03	.641202E+00	.185538E+00	-.323228E+02	.232940E+02	.529318E+02	7
8	8.0105	.533971E+02	.443992E+03	.791602E+00	.126738E+00	-.201056E+02	.287578E+02	.617537E+02	8
9	10.0896	.325687E+02	.379379E+03	.926556E+00	.834340E-01	-.126108E+02	.336605E+02	.705757E+02	9
10	12.8172	.191469E+02	.339070E+03	.103692E+01	.518511E-01	-.772865E+01	.376697E+02	.793977E+02	10
11	16.5906	.107751E+02	.314941E+03	.111657E+01	.302672E-01	-.472768E+01	.405636E+02	.882196E+02	11
12	21.9252	.617826E+01	.302252E+03	.116362E+01	.177128E-01	-.309734E+01	.422726E+02	.970416E+02	12
13	28.8986	.415070E+01	.296882E+03	.118476E+01	.120064E-01	-.238384E+01	.430405E+02	.105864E+03	13
14	36.6702	.340480E+01	.294981E+03	.119243E+01	.988031E-02	-.212297E+01	.433192E+02	.114686E+03	14
15	44.3431	.314326E+01	.294338E+03	.119505E+01	.913129E-02	-.203198E+01	.434144E+02	.123507E+03	15
16	51.6685	.304775E+01	.294110E+03	.119598E+01	.885723E-02	-.199892E+01	.434482E+02	.132329E+03	16
17	58.6048	.301166E+01	.294027E+03	.119632E+01	.875360E-02	-.198647E+01	.434607E+02	.141151E+03	17
18	65.2400	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.434647E+02	.149973E+03	18

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.22492E+00	.50940E-01	.13927E-01	.53772E+00	.16955E+00	.36602E-03	.66795E-03	1
2	.76580	.21640E+00	.26531E-01	.60640E-02	.56481E+00	.17965E+00	.46492E-03	.21430E-02	2
3	1.59460	.16485E+00	.16982E-02	.35128E-03	.63132E+00	.15177E+00	.46673E-04	.22319E-02	3
4	2.58433	.99050E-01	.25953E-03	.16392E-04	.69592E+00	.91414E-01	.12021E-05	.25361E-03	4
5	3.67641	.55988E-01	.18069E-02	.62228E-03	.73534E+00	.50657E-01	.33828E-07	.67960E-06	5
6	4.91710	.32200E-01	.22370E-02	.94178E-03	.75720E+00	.28611E-01	.29983E-10	.13370E-08	6
7	6.32882	.18993E-01	.20795E-02	.94100E-03	.76973E+00	.16602E-01	.30201E-13	.47274E-11	7
8	8.01054	.11240E-01	.16922E-02	.79803E-03	.77740E+00	.97160E-02	.58930E-16	.26315E-13	8
9	10.08959	.64622E-02	.12404E-02	.60190E-03	.78235E+00	.55860E-02	.27323E-18	.29197E-15	9
10	12.81720	.34579E-02	.80777E-03	.40062E-03	.78563E+00	.30659E-02	.31693E-20	.75441E-17	10
11	16.59061	.16313E-02	.44969E-03	.22705E-03	.78773E+00	.15818E-02	.81451E-22	.44050E-18	11
12	21.92523	.65336E-03	.20764E-03	.10642E-03	.78891E+00	.81198E-03	.40983E-23	.54566E-19	12
13	28.89857	.23195E-03	.83184E-04	.43163E-04	.78944E+00	.49007E-03	.34326E-24	.12054E-19	13
14	36.67017	.80165E-04	.31720E-04	.16620E-04	.78964E+00	.37731E-03	.39067E-25	.36687E-20	14
15	44.34315	.27963E-04	.11921E-04	.62911E-05	.78971E+00	.33952E-03	.50332E-26	.12660E-20	15
16	51.66853	.92256E-05	.41328E-05	.21912E-05	.78973E+00	.32628E-03	.58270E-27	.42383E-21	16
17	58.60479	.22416E-05	.10273E-05	.54583E-06	.78974E+00	.32144E-03	.35450E-28	.10408E-21	17
18	65.23998	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	18

MOLE FRACTIONS

PT	Y/R	O	O2	K	KOH	KO2	HO2		PT
1	0.00000	.13158E-04	.17573E-03	.58197E-03	.11404E-02	.14053E-07	.42324E-07	0.	1
2	.76580	.11998E-03	.22158E-02	.48220E-03	.11280E-02	.92910E-07	.42180E-06	0.	2
3	1.59460	.22183E-03	.46308E-01	.98599E-04	.10987E-02	.72977E-06	.22273E-05	0.	3
4	2.58433	.24432E-04	.11234E+00	.39262E-05	.70995E-03	.72970E-06	.16248E-05	0.	4
5	3.67641	.26033E-06	.15516E+00	.59177E-07	.40074E-03	.70912E-05	.23373E-04	0.	5
6	4.91710	.70042E-09	.17855E+00	.38192E-10	.23091E-03	.78889E-05	.19004E-04	0.	6
7	6.32882	.15767E-11	.19149E+00	.98526E-14	.13655E-03	.70852E-05	.13870E-04	0.	7
8	8.01054	.30454E-14	.19906E+00	.35362E-17	.81067E-04	.56718E-05	.94679E-05	0.	8
9	10.08959	.51244E-17	.20370E+00	.65413E-20	.46783E-04	.41153E-05	.60370E-05	0.	9
10	12.81720	.77894E-20	.20661E+00	.45568E-22	.25142E-04	.26583E-05	.34991E-05	0.	10
11	16.59061	.14976E-22	.20837E+00	.68428E-24	.11921E-04	.14684E-05	.17611E-05	0.	11
12	21.92523	.21295E-24	.20931E+00	.16960E-25	.48013E-05	.67257E-06	.74400E-06	0.	12
13	28.89857	.15845E-25	.20971E+00	.65743E-27	.17148E-05	.26721E-06	.27584E-06	0.	13
14	36.67017	.17986E-26	.20986E+00	.50917E-28	.59615E-06	.10110E-06	.98600E-07	0.	14
15	44.34315	.24265E-27	.20991E+00	.99586E-29	.20901E-06	.37750E-07	.35244E-07	0.	15
16	51.66853	.37509E-28	.20992E+00	.29440E-29	.69217E-07	.13028E-07	.11812E-07	0.	16
17	58.60479	.13487E-28	.20993E+00	.70710E-30	.16848E-07	.32316E-08	.28906E-08	0.	17
18	65.23998	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	0.	18

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